Australian Government

The first 10 years of the

Bragg Institute

2002 - 2012

Cover image:
Laue Diffraction image from NiAl

shape-memory alloy taken on the

KOALA Laue Diffractometer

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QUOKKA and OPAL's neutron guide hall 2010

Foreword

It is a great pleasure to introduce this wonderful compilation of the achievements of the Bragg Institute during its first 10 years, told by the people who were involved in developing the Institute from its very beginnings.

In 2013, ANSTO is celebrating its 60th anniversary. The achievements of our organisation over the past six decades have been bolstered tremendously by the many successes of our Bragg Institute.

ANSTO's Bragg Institute has established itself as one of Australia's most significant scientific user platforms, with seven operating neutron beam instruments having been successfully constructed and commissioned, with a further six instruments under development. The Institute has also established a world-leading National Deuteration Facility that supports specialised research based on the distinct neutron scattering from hydrogen and deuterium.

Researchers from 137 Australian and international research organisations have used the neutron beam instruments over the past 10 years, with over a thousand research articles being published in a range of high-quality journals. Enabled by OPAL, one of the world's most modern research reactors, Bragg is well placed to continue to support research for many more decades to come.

I trust you will enjoy the individual stories of the people behind developing, installing and running the instruments. They have shared their achievements, challenges and insights for the exciting future that is ahead for the Bragg Institute.

I wish to extend my appreciation to our users and collaborators for their ongoing support. Although it is sometimes inappropriate to single out individuals, I want to extend my personal thanks to Rob Robinson, who has built and steered the Institute over the first decade.

I congratulate all of our people, both past and present, who have contributed to the success of the Bragg Institute.

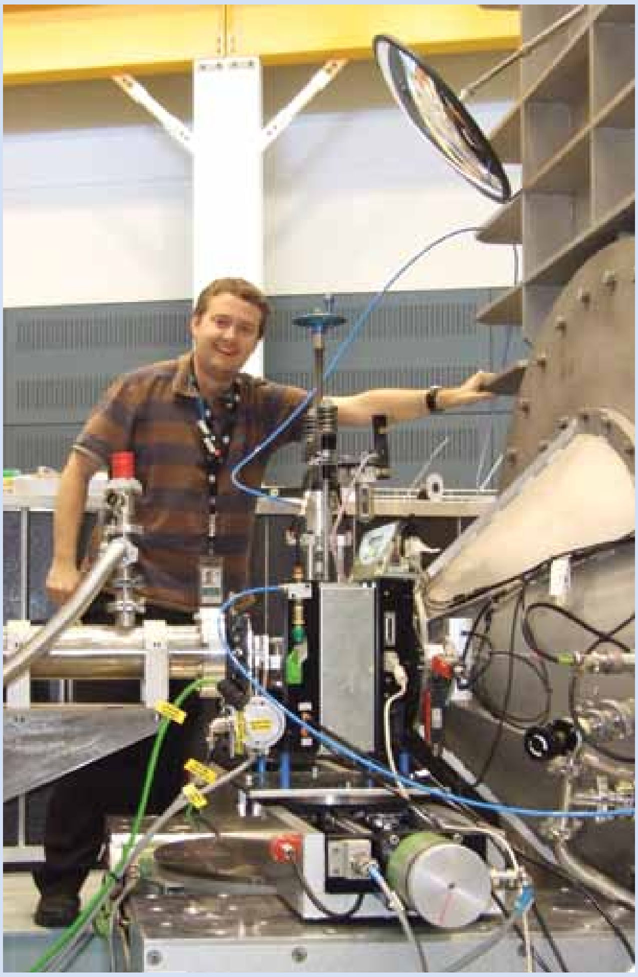
Dr Adi Paterson

Chief Executive Officer

Australian Nuclear Science and Technology Organisation

The Bragg Day Out, Como Hotel, March 2003.

The Bragg Institute in 2010



James Doutch experimenting on QUOKKA

Showing Attorney General Philip Ruddock around in 2007

John Daniels doing electronic-field experiments on TASS at HIFAR

Bragg's Technical Support Group (L-R) Matt Bell, Merv Perry, Marty Jones, Alain Brule

Rob Robinson, former CEO Helen Garnett and Bill Stirling

We had to build a reactor to support world-class neutron beam science

ANSTO: A supportive centre of excellence in beam-line instruments and their applications for the 21st century

Helen Garnett PSM (ANSTO CEO at the time the Institute was formed)

The seed for the concept that Australia should be a centre of excellence in neutron and X-ray beam science was sown 10 years before the launch of the Bragg Institute in December 2002.

In late 1992 the Research Reactor Review - sometimes known as the McKinnon Review - was launched. HIFAR was aging and its design and safety systems were unlikely to enable it to operate into the 21st century. The push for a new reactor was mounting. Also in 1992, the 'Australian' X-ray beamline project was launched at the Photon Factory in Japan.

During the preparation of ANSTO's submission to the McKinnon Review, which I led as the then Deputy Executive Director, multiple lines of evidence attested to the historic strength of Australian neutron scattering and its contribution to condensed-matter science: a strength that had been underpinned by a reactor and beam-line instruments that were once world class. By 1992, HIFAR was now old and the neutron beam instruments, while being renewed somewhat through the AINSE consortium, had to a large extent lost their usefulness and appeal to younger scientists. The action for both neutron and X-ray beam science was overseas: Australians had been forced to adopt suitcase science.

Australia needed a new research reactor for its medical radioisotope supplies, but as the McKinnon Review progressed, my view firmed that an isotope reactor alone would be an inappropriate investment - we had to build a reactor to support world-class neutron beam science, one with multiple instruments and a cold source. We had to be able to support the soft-matter science in which Australia had considerable research effort and the emerging nanosciences. Our opponents, the antinuclear activists - were however claiming that neutron scattering had had its day and that synchrotrons with their X-ray beams could do it all. These claims did not resonate with the claims by eminent scientists within and outside ANSTO and international consultation just reaffirmed the complementarity: ideally Australia should have on-shore access to both a world-class research reactor and a quality synchrotron.

Given the multipurpose nature of a research reactor, replacing HIFAR was ANSTO's first priority - a synchrotron had to be a later goal. Following the release of the McKinnon Report in 1994 and through till 1997, the case for a replacement research reactor - OPAL - was painstakingly built with ANSTO's stakeholders, with political parties and with the politicians. During this period, visits to leading neutron scattering institutes and synchrotron facilities around the globe were added onto my other overseas commitments as Chief Executive. An understanding of how the best facilities operated was gained: there needed to be dedicated teams with a focus on the instruments, the scientific disciplines they supported and the users - many of whom would, and should be from outside of ANSTO, whether in other research organisations, in universities or in industry. It became apparent that the ANSTO divisional approach - focused on ANSTO's business would not be the correct model for a 21st century world-class user facility.

But first we had to get the facility and all efforts had to be on achieving Federal Government commitment to a new research reactor. With the commitment to funding, announced on September 3 1997, the detailed planning for OPAL began, a Beam Facilities Consultative Group was established and a myriad of complementary processes were triggered - Environmental Impact Assessment, Public Works Committee review and more. With these processes satisfactorily completed, we were finally able to recruit staff to lead the neutron beam instrument project. After an international search, aided by the commitment of international colleagues, Dr Rob Robinson was recruited as the Leader of the Neutron Scattering and Synchrotron Radiation Research Group in 1999.

By this time ANSTO staff were also supporting Australian synchrotron users, not only in Japan but also at the Advanced Photon Source in the USA and ANSTO staff were joining with other scientists in Australia to promote a synchrotron as a facility that should be considered for funding in the next Major National Research Facilities (MNRF) funding round. I gave talks to the numerous groups, including the

ANSTO: A supportive centre of excellence in beam-line instruments and their applications for the 21st century

Helen Garnett PSM

Australian Vice Chancellors group, Commonwealth Committees and briefed the then Minister for Science Nick Minchin on the complementarity of the reactor and a synchrotron. Early in 2000 the Federal Government announced that there would be a competitive process for funding large scientific facilities through a Major National Research Facilities round, with decisions in 2001. Quietly I saw the opportunity to achieve my vision for an Australian synchrotron co-located with the new research reactor at Lucas Heights. With the tendering process for the new research reactor almost complete, effort swung to convincing the New South Wales Government to support a bid for the synchrotron at Lucas Heights.

The New South Wales Government had been quietly supportive of the new research reactor project and its potential contribution to make New South Wales a scientific centre of excellence. It seemed reasonable to believe they would be supportive of the concept to make Lucas Heights an even bigger player in national and international science - but it would take a commitment of significant funding from the state and support from scientists in other jurisdictions that were not likely to compete. Thus began a series of discussions with key players including Professor Brian O'Connor from Western Australia. We were all unanimously of the view that any facility at Lucas Heights would need to be distinguished from ANSTO's own business. With a concept in mind we achieved a meeting with senior NSW officials in April 2000.

While emphasising our vision for the two facilities co-located at Lucas Heights and how it could be 'the' place, Brian came out with the suggestion that an appropriately distinguished name was the Bragg Institute, named after Australia's first Nobel Laureate, William Lawrence Bragg. The NSW Government did eventually agree to support a NSW bid for the synchrotron at Lucas Heights and a detailed submission prepared. However, with the decision by the Victorian Government to build the Australian Synchrotron, the concept of the Bragg Institute being 'the' name of the Neutron Scattering and Synchrotron Radiation Research Group at ANSTO retained momentum. There was support external to ANSTO

Birds-eye view of OPAL and the Neutron Guide Hall, behind it, during construction

and within ANSTO. There was no doubt in my mind that the group had to be separated from Physics Division and given the direct responsibility for project managing the instruments for the new reactor and building ANSTO's partnerships, and reputation, with the neutron beam user community. Discussions were held with the Director, Physics Division, who was then on secondment to the IAEA in Vienna. With his understanding, the concept was put to the ANSTO Board during 2002. And so in October 2002, the announcement was made that the Bragg Institute would be launched later that year. Since December 2002, the team, led by Rob Robinson has built on its excellent work in the years 1999-2002 and Australian science has benefited significantly from the ingenuity and commitment of all associated with the Bragg Institute.

Ten years is a long time in some ways - but a short time in the life of an institute aiming to be a world leader. Continued commitment to excellence and partnership will no doubt ensure that the second decade in the life of 'the Bragg' will build further on the vision sown back in 1992 - ANSTO hosting a world-class centre of excellence in neutron, and X-ray science.

Bragg Institute 10th birthday

John White, Australian National University

The Replacement Research Reactor (now called OPAL) funded by the Commonwealth Government in 1997 has placed Australia in the forefront of radioisotope production and nuclear technology in the Asia-Oceania region. The Bragg Institute, established in 2002 has done the same thing in neutron scattering science and technology. It is a pleasure for all who have benefited from the remarkable suite of instruments installed since then, to wish the Institute a very happy 10th birthday. ANSTO and the Australian scientific, engineering and medical communities now have at their disposal a landmark facility. What should be a scientific goal of this investment? A goal of the Asia-Oceanic Neutron Scattering Association (AONSA) is part of the answer:

The gestation process for these facilities was long. The realisation in 1985 by Professor John Carver's submission to the Australian Science, Technology and Engineering Council (ASTEC), that the Lucas Heights facilities were far behind those available in Europe and the United States in many areas, led to the first "suitcase scientists" doing work overseas not possible at home. The lack of a cold neutron source was of paramount concern since great advances in 'soft matter', polymer, colloid and biological sciences in Europe could not be matched in Australia. High respect is due to Australian 'hard matter' science with the diffraction instruments at the HIFAR reactor (Australia's now retired research reactor).

The Australian Academy of Science through the National Committee for Crystallography played a key role advising the Federal Government from 1990 onwards.

My own vision of this project is that of a bipolar development of resources with our Asian neighbours. We must have a replacement reactor capable not only of the irradiation and isotope production needs of the next twenty or thirty years, but also one which will place Australia again (as in 1958) at the forefront in neutron scattering work for the foreseeable future - at least in some scientific and technological areas…

…the desirability for eventual, if not immediate international collaboration and competition in the exploitation of central facilities.

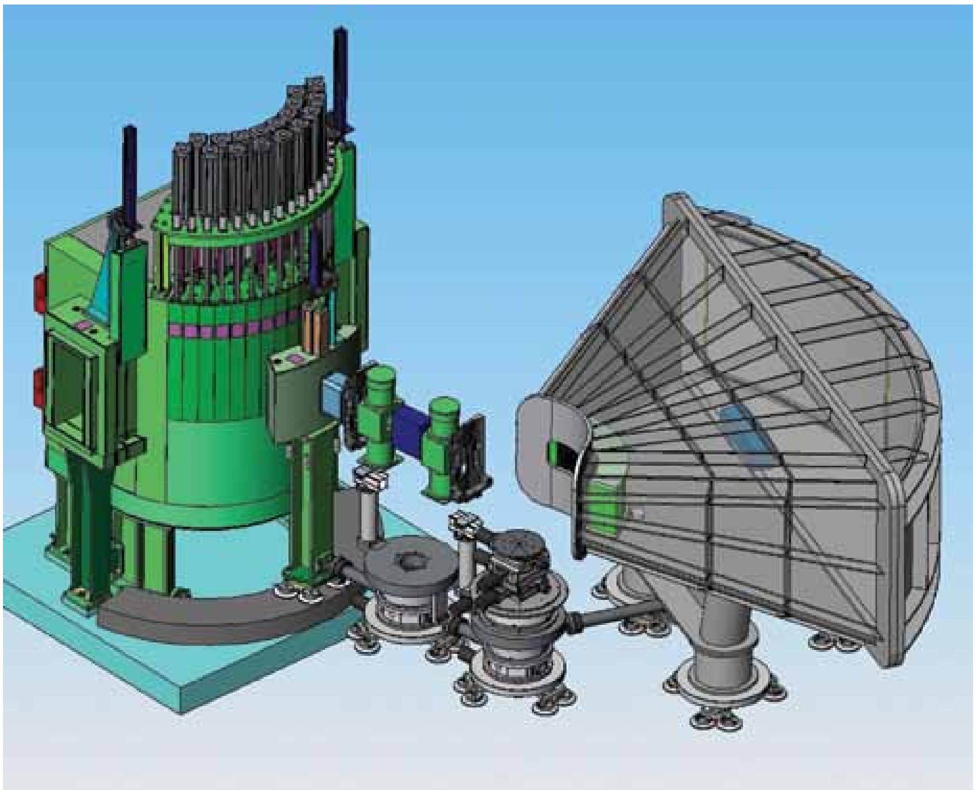
(John White in letter to Prof D.P.Craig President of AAS 15 October 1992)

With the report of the Mackinnon Commission (1993) and the updated report to the Senate Review (1998) all of the struggles to install a cold source in the HIFAR reactor came to an end. A scientific brief for new neutron scattering instruments – developed over a number of years in close consultation with the Australian science community adopted a guiding principle along the lines:

That no instrument should be constructed unless its performance could at least match the best overseas performance.

This salutary challenge was taken up for reactor design and neutron instruments. It was a reasonable challenge for a new initiative to profit from the best of the many remarkable developments in neutron scattering technology overseas in the 1970s, 1980s and 1990s. Thus optimised moderators, neutron beam guides and top of the mark detectors and monochromators were studied and incorporated.

That no instrument should be constructed unless its performance could at least match the best overseas performance



Schematic diagram of the PELICAN time-of-flight spectrometer

The outcomes since 2005 show instrumentation performance of the highest international quality and illustrate how well the Australian designers and overseas constructors have responded.

A second feature of the design was that the reactor beam hole configuration should allow a future second cold source and neutron guide hall for cold beam neutron instruments.

The Bragg Institute is to be congratulated on having the first meeting (in 2012) to begin planning to realise this in the next ten years.

Why is it important? In 2003-2004 the high attendance of user meetings, subsequent proposed demand, and international interest in small-angle scattering reflectivity and time-of-flight spectroscopy measure the quality of Australian and Asia-Oceania science needing these facilities.

Complementarity of new Bragg instrumentation to new facilities in Asia-Oceania should be the watch-word for the next step at the Bragg Institute. Its international recognition through publications over the last five years and the scientific collaborations formed across the world point to this policy. Competitive provision for the Australian scientific community intersected with that of others in our region on a trading basis for access will produce a high contribution to the Australian national interest as has the provision of isotopes and nuclear expertise. The achievement over 20 years can be as high as that of the Institut Laue Langevin in Europe.

Origins of the ANSTO Bragg Institute

Brian O'Connor, Curtin University

The Bragg Institute in 2006

The ANSTO Bragg Institute was launched in December 2002 under the leadership of Dr Rob Robinson who had arrived at ANSTO in December 1999 to take up an appointment as Leader of the ANSTO Neutron Scattering and Synchrotron Radiation Research Group. Rob's appointment came at a time of great strategic significance for Australian science, with ANSTO signing a contract with the Argentinian company INVAP S.E. on 13 July 2000 to design and construct the OPAL reactor; and with the Commonwealth of Australia calling for bids for siting an Australian synchrotron.

The New South Wales (NSW) bid for hosting the synchrotron was led by Prof Helen Garnett, with the vision that there would be much merit in co-locating the new synchrotron and the planned replacement reactor. The vision was to develop a research entity at Lucas Heights which would optimise the very strong synergies between neutron scattering and synchrotron radiation applications.

ANSTO's initial engagement with NSW government officers on the NSW bid took place at a meeting in Sydney's CBD in early 2001. Prof Garnett was accompanied by Dr Robinson and Prof Brian O'Connor of Curtin University of Technology who had chaired the ANSTO 'Strategic Planning Committee on Neutron Beam Applications for the Future – Facilities for Australians'. At this meeting, a schematic design was presented to establish a national research institute at Lucas Heights which would serve as a focus for Australian research involving the use of neutron scattering and synchrotron radiation. The concept to call the institute the Bragg Research Institute was proposed at that meeting by Prof O'Connor.

Regrettably, consideration of the NSW bid to host the synchrotron, along with bids from Queensland and the Australian Capital Territory (ACT), was abandoned by the Commonwealth when the Victorian Government announced in June 2001 that it would design and construct the synchrotron in Melbourne. Notwithstanding this development, ANSTO refined the Bragg Institute concept and subsequently decided that the neutron scattering operation for the OPAL reactor would be named the Bragg Institute. Since then the Bragg Institute has successfully led the development of world-competitive neutron scattering science in Australia, and has also given much impetus to Australian synchrotron radiation research.

First Meeting of Bragg Institute Advisory Committee in March 2003 – outside Building 58: left to right: Shane Kennedy, Richard Garrett, Rob Lamb, Evan Gray, Brian O'Connor, George Collins, Alan Leadbetter, Barry Muddle, Rob Robinson, Don Napper

Reflections on 10 years with the Bragg Institute

Rob Robinson

On 14th October 2002, ANSTO Chief Executive Officer, Helen Garnett, summoned the staff of ANSTO's Physics Division to an "all-hands" meeting in the AINSE Auditorium. After 90 minutes, she announced the formation of the Bragg Institute, a new initiative for ANSTO, and the audience (or at least a large part of it) erupted into applause. Of course, some were saddened by the passing of the old ANSTO Physics Division, and openly wondered how a nuclear organisation could conceivably manage without one. But not the multi-disciplinary team of neutron scatterers! At the time, the Neutron Scattering and Synchrotron Radiation Group comprised around 40% of the Physics Division, though we were probably seen by some as the black sheep, hidden away behind HIFAR's barbed-wire security fence. But with the OPAL construction project, the group had already started to grow substantially, in preparation for ANSTO's new research reactor.

I had known for some weeks previously that Helen was going to make this announcement, and had wondered for some time prior to that what would happen in the scenarios that Claudio Tuniz (who had hired me in 1999, while Director of Physics) would or would not return from a 3-year secondment to the International Atomic Energy Agency in Vienna. But I had not expected this particular idea. Anyway, I think that Helen must have been quite nervous on the day, as she spoke for well over an hour before getting to the main point – I kept thinking "Helen – please give them the punchline!", as I knew what was coming. Change is never easy. But in the end, the reaction was quite benign.

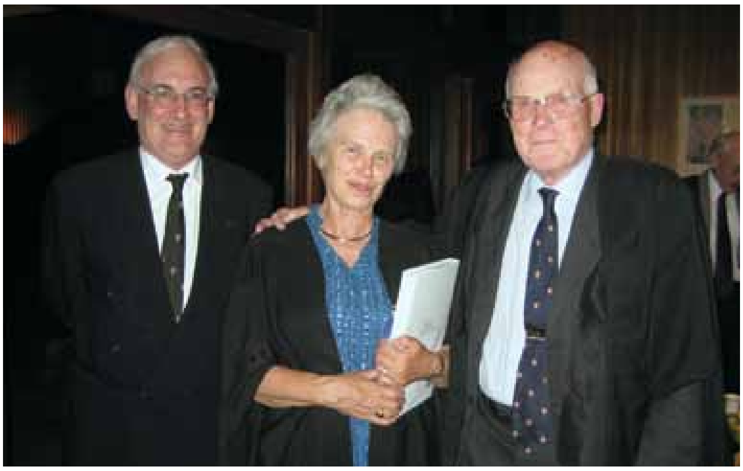
The next step was to decide which of the admin and support staff would come with us, and which would go with the accelerator group to the Environment Division. In the end, Kevin Morrison joined us as a business manager from ARI, Judy Penny continued to support us with procurements in the Neutron Beam Instruments Project, and we were lucky to get Cherylie Thorn as Group Secretary. The staff of the Australian Synchrotron Research Program also moved up to the complex of buildings and transportables that formed B58.

We were not to be a "Division" in its own right, but rather were under the wing of the Materials Division, which was led by George Collins, and who represented us on the Senior Management Committee. This arrangement was dubbed the "umbilical chord", reflecting the initial dependence and nurturing from Materials, but also the sense that we would eventually grow into an independent adult. We were and are eternally grateful to George Collins for his patient help and mentoring, which has persisted long after the umbilical was cut.

It was a deliberate choice for us to be an "Institute" rather than a "Division", and some ANSTO Board members were apparently concerned about the elitism that this implied. But it also reflected the much stronger emphasis on partnership with other organisations, and indeed our by-line was "ANSTO in Partnership", reflecting ideas for a virtual institute spanning all of Australia, and covering both neutrons and synchrotron radiation. Another early task was to come up with a suitable logo for the Institute, and a competition was held amongst the staff. Eventually we selected an idea from Darren Goossens (then a postdoctoral fellow, but now at the Australian National University), consisting of a large upper-case "B" for Bragg, but as a set of interfering circular waves, as in the classic Young's Slits Experiment (see page 16). The colour and artwork were refined by ANSTO Communications, and we used it on our webpages, presentations and business cards for several years, until the Howard Government issued a decree banning such sub-branding and enforcing a regimen of strong and standardised Australian Government branding with the national coat of arms.

At the time, we were organised into five groups, as shown below. Those staff in red were about to join us: Dehong Yu (from University of Western Australia, as instrument scientist for LONGPOL), and Andrew Nelson and Kia Wallwork as postdoctoral fellows. Of course, Andrew is now one of our leading soft-matter researchers, an instrument scientist for PLATYPUS, and a contributor to this book, while Kia is in a leadership position at the Australian Synchrotron in Melbourne. Vanessa Peterson, another contributor

The data acquisition team



With Lady Lucy Adrian and Stephen Bragg in Cambridge in 2007

to this volume, was in 2002 a graduate student based with us – after graduating she did a postdoc in the United States, before returning to us as a staff member on our powder-diffraction team. Twelve others are still with the Institute after 10 years of continuous service. Three of our staff from 2002 now work for the Australian Synchrotron, a number have leadership positions at other overseas neutron sources, and some have moved elsewhere within ANSTO.

Another early task was to set up the Bragg Institute Advisory Committee. Helen was very keen on this idea, though surprisingly this approach has not been copied elsewhere within ANSTO, despite being common practice in other nuclear organisations overseas. The members of the committee are listed in Appendix 1, and Don Napper (Sydney University) was the inaugural chair. For most of the Institute's life, at least when we have been managing tens of millions of dollars of capital programs, the Beam Instruments Advisory Group has also advised us, under the chair of Tony Klein (University of Melbourne) and later Dan Neumann (NIST). Finally, a third external committee, the Program Advisory Committee advises us on the allocation of neutron beam time and deuteration resources. The Program Advisory Committee came into existence once OPAL went critical in 2006, and includes representatives of the Australian Institute of Nuclear Science and Engineering, the Australian Neutron Beam Users Group and the National Science Council of Taiwan, along with a number of external ANSTO nominees. It has been chaired successively by Jill Trewhella (Sydney University), Calum Drummond (CSIRO) and Anton Middelberg (University of Queensland).

Another key set of relationships have been with other parts of ANSTO. Of course, the Institute is co-located (joined at the hip) with Reactor Operations, and we occupy a common set of buildings, and have overlapping regulatory obligations. In fact, the Institute is completely and absolutely dependent on Reactor Operations for a reliable supply of both cold and thermal neutrons. In 2006, before OPAL went critical, Greg Storr (Head of Reactor Operations) and I negotiated a Service Level Agreement, delineating who is responsible for what and identifying key interfaces. This has worked reasonably well. The Institute has also had consistently strong scientific collaboration with ANSTO's Materials Division, which then morphed into the Institute of Materials and Engineering Sciences, and has now been re-branded as the Institute of Materials Engineering. Finally, there is a large number of engineering, design and draughting staff seconded from ANSTO-Engineering into the Institute. Mostly this was short-term, but Alain Brule has been with us continuously since 2002. We have also drawn heavily from the talent pool in ANSTO's excellent apprenticeship program, to source technicians.

Of course, we also have important interactions with all the other parts of ANSTO, and we thank our colleagues in these divisions for all of their support over the past 10 years.

A selection of key milestones in the Institute's life so far is given in the appendices, and I would like to highlight a couple of important events in late 2005: the hosting of the 2005 International Conference on Neutron Scattering in Sydney; and the "Blue Mountains Workshop", held at the Hydro Majestic Hotel in Medlow Bath immediately afterwards. Around 750 attendees came to ICNS2005, and it was the first time this meeting had been held outside of Europe, North America or Japan. We had the chance to highlight our science and aspirations, and to show our presence on the world stage. Overseas friends still reminisce about how they first came to Australia

Bragg Institute Organisational Chart from March 2003, including secondments from ANSTO-Engineering.

Staff who were about to join us are listed in red.

Bragg Institute

Leader – Rob Robinson

Neutron Scattering
Leader: R Robinson

- R Robinson
- M M Elcombe
- S J Kennedy
- R B Knott
- G E Gadd
- L Cussen
- M James
- R Piltz
- W Klooster
- E Gilbert
- M Hagen
- J Schulz
- O Kirstein
- D Yu

Synchrotron Radiation Group
Leader: R F Garrett

- R F Garrett
- D J Cookson
- G J Foran
- A Stampfl
- J Hester
- H Tong
- C Harland

Scientific Operations Group
Leader: B Hunter

- B Hunter
- P Baxter
- A Studer
- Yang Fei
- N Hauser
- M Prior
- P Hathaway
- M TranC

Business Management Support Group
Leader: K Morrison

Business Manager:	K Morrison
Assistant Business Manager:	J A Penny
Admin. Assistant:	C Thorn
Admin Support (ASRP)	M Edmondson

Technical Support Group
Leader: D Penny

- D Penny
- M Perry
- M Jones
- M Bell

NBI Engineering Team

- S Kim
- A Brule
- G Horton
- R Moore
- T Noakes
- E Imamovic

Post Docs

- C Garvey
- D Goossens
- D Sutton
- A Nelson
- J Connolly
- K Wallwork (ASRP Fellow)

Students

- V Peterson
- P Smythe
- T Young

bragg institute

ansto in partnership

The 2005 International Conference on Neutron Scattering in Sydney

for this meeting, and it even influenced some of our present staff to join us. The Blue Mountains Workshop really set our course for expansion, and the vision produced there has been realised to a great extent with the Neutron Beam Expansion Project, described by Frank Klose and Paris Constantine later in this book. A number of leaders from other neutron sources, including Thom Mason (Oak Ridge), Winfried Petry (Munich) and Feri Mezei (Berlin) attended.

In fact we are also grateful to all of our friends and colleagues in other neutron and synchrotron sources around the world. In part this is because, collectively, our staff have had the privilege of working at almost all of the leading centres in Europe and the USA, prior to joining ANSTO, and therefore retain strong networks around the world. We are particularly grateful to our friends at NIST, for their tireless advice, help and mentoring, and at the Institut Laue Langevin in Grenoble (with its large cadre of Australian crystallographers, and huge effort in advancing neutron technology), but in truth we have benefitted from advice, technology transfer and ideas from all of the leading international centres. We like to think that we are now giving something back, particularly in the Asia-Pacific region, and to NECSA in South Africa, and we are proud that we are now seen as a significant player in the world-wide "neutron family."

Finally, we have been privileged to have had some direct contact with the Bragg family, after whom we are named. Initially, the contact was through Prof. Tony Kelly, Lawrence Bragg's last graduate student in the physical sciences, whom I met at a conference in Sydney in 2006 He introduced me to Lawrence's eldest son Stephen, and to his niece Lady Lucy Adrian, a granddaughter of William Henry Bragg. My wife and I were privileged to have dinner with them in Cambridge in 2007, and our library now features a letter written to us by Stephen Bragg. Of course, the Australian research community was well aware that 2012 would be the centenary of "Bragg's Law" for X-ray diffraction from crystals, which applies in exactly the same way to neutron and electron diffraction. In order to celebrate this, in December 2012, we helped to organise a special Centenary Meeting in Adelaide, Lawrence Bragg's birthplace, involving other members of the family and scientific leaders from around the world. The background to this is beautifully described in John Jenkins's article in this book. But it is a happy confluence of events that we celebrate the Bragg Institute's tenth birthday, just as Australia celebrates its first Nobel Prize, awarded to the great physicists after whom we are named, and in whose footsteps we still tread.

Bragg's Law: 100 years on and still going strong

John Jenkin, La Trobe University

The Bragg family in Adelaide, circa 1902, (L to R) Lawrence, Gwendoline, Bob and William (Courtesy, Dr S.L. Bragg)

Introduction

On 11 November 1912, (William) Lawrence Bragg announced his discovery of Bragg's Law and his solution of the first crystal structure. These discoveries have led to the electronic and computer revolution, the analysis of the rocks brought back from the moon, the current revolution in medical science, and much else besides. In celebrating its 2012 centenary, we should acknowledge Lawrence Bragg as one of the greatest scientists of the twentieth century and one of Australia's greatest sons.

Lawrence Bragg is also still the youngest person ever to win a Nobel Prize: for Physics in 1915 with his father. At its jubilee, Lawrence delivered the first Nobel Guest Lecture at the 1965 Nobel ceremonies in Stockholm, and he began as he had done innumerable times before: "It is sometimes said that my father and I started X-ray analysis together, but actually that was not the case"; and he went on to point out that, as a research student at Cambridge, he alone had first analysed the Laue photographs using a reflection model, that he alone had devised Bragg's Law, and that he alone had thereby determined the first crystal structures, of zincblende (ZnS) and the alkali halides.

The journey to Bragg's Law

Late in 1885, persuaded by his Cambridge friend and tennis partner J.J. Thomson, William Henry Bragg applied for the vacant Elder Chair of Mathematics and Experimental Physics in the University of Adelaide. At the interviews, a committee of which Thomson was Chairman, selected William. Aged just 23, he had graduated BA with first class honours in mathematics, but he had never devised a university course nor taught in one, and he had done no research.

On his first day in Adelaide, William was taken to meet the senior scientist in the colony, Charles Todd and his family; but it was their third daughter, Gwendoline, that caught his eye. They fell in love, were married three years later, and three children were subsequently born in Adelaide: Lawrence in 1890, then Robert (Bob), and later a daughter, Gwendy.

Lawrence Bragg, Cambridge research student, circa 1913, soon after his discovery of Bragg's Law and his invention of X-ray crystallography (Courtesy, Dr S.L. Bragg)

William's teaching, public lectures and research slowly blossomed, and he became a world authority on the alpha-particles from radioactive decay. This was followed by an investigation of the nature of X- and gamma-radiation, in which he suggested, in contrast to most European scientists, that it was composed of neutral particles.

Lawrence and Bob were educated at St Peter's College in Adelaide, where Lawrence was promoted to higher and higher grades; he was just 14 years old in the sixth form with other students aged 17 and 18. This unhappy disjunction continued at the university, where he studied in his father's office and where he topped most of his classes, many taught by his father. He graduated BA at age eighteen, with first-class honours in mathematics, only weeks before the family sailed for England: William to the physics chair at Leeds, Lawrence to further mathematics at Cambridge.

A year later, encouraged by his father, Lawrence changed to physics and again graduated with a first. He entered the Cavendish Laboratory but was disappointed by the research project J.J. Thomson offered him, and he happily joined the family on the Yorkshire coast for the summer holidays of 1912. Here, he and his father read a letter from Germany reporting the Laue experiment that showed that X-rays could be diffracted. But it was also clear that Laue's analysis of the results was incomplete; he assumed that fluorescent radiation from a crystal of simple cubic geometry was responsible for the non-circular spots on the photographic plate.

William returned to Leeds to try to salvage his particle model of X-rays; Lawrence returned to Cambridge to try and find a better explanation. Using insights provided by his undergraduate lectures and advice about possible crystal structures, Lawrence envisaged a reflection of the incident radiation from atoms in a face-centred-cubic structure, leading to elliptical diffraction spots that precisely reproduced the German data. He presented his findings to the Cambridge Philosophical Society, which soon published them. Lawrence then used his new understanding to discover the structures of several alkali halide crystals.

Using a crystal of known structure, father William now used the technique to study X-rays, until Rutherford in Manchester bullied him out of it in favour of Harry Moseley. William then turned his new spectrometer to the study of crystals, and father and son, together and separately, plundered the new field. Lawrence recalled, "we had a wonderful time … discovering a new goldfield where nuggets could be picked up on the ground … until the war stopped our work together".

Lawrence's subsequent career

It was now 1915 and The Great War was in full swing. For more than four years, close to the front line, Lawrence developed the science of 'sound-ranging' to locate the big German guns, and in 1917 and 1918 this played a major role in the drive for Allied victory in the First World War, a story still to be adequately told. Lawrence Bragg should be acknowledged as a war hero as well as a superb scientist!

Here we may simply note that in 1915 the family's Nobel Prize could not be celebrated: because of the war and because his brother Bob and Lawrence's closest friend had both been killed. His father's internationalism was damaged, his mother's mourning was deep and long lasting, and Lawrence's equanimity was threatened by the horrors of the Western Front. Appointed post-war to Rutherford's Manchester chair, Lawrence suffered a nervous breakdown, overcome when his research blossomed, he was made a Fellow of the Royal Society and he married the bubbly Alice Hopkinson.

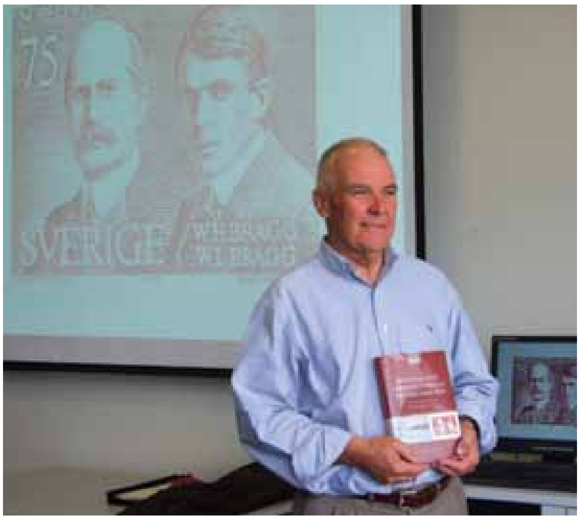
Lawrence's research resumed. He and his 'Manchester School' began a long and successful program to determine the structures of silicate minerals, he wrote a new book, *The Crystalline State*, and he launched a new study of metals, alloys, and alloy phase diagrams. In a lecture to the Royal Society of Edinburgh in 1935, he mentioned the attraction of "an X-ray investigation of structures produced by living matter", and that it might be "the most interesting field of all".

In 1937 Lawrence again succeeded Rutherford, this time in the Cavendish chair at Cambridge, where the reception was again cool. Many said a crystallographer wasn't a real physicist at all! But again Lawrence triumphed. As Brian Pippard said later, "when one looks back on Bragg's tenure … [it] came to fruition in advances … that even eclipsed any from Rutherford's Cavendish". He was no doubt thinking of the Nobel Prizes awarded to Crick, Watson, Kendrew and Perutz in 1962, and later to Ryle.

Finally, Lawrence Bragg accepted another poisoned chalice at the Royal Institution of Great Britain in London, where he reorganised its dysfunctional administration, introduced successful lectures for school children, gave discourses that were televised for the first time, and saw his research blossom yet again. He died on the first of July 1971.

Conclusion

The Braggs took science to the public, they supported schoolteachers and schoolchildren, they recruited women staff and female research students, and, above all, they breached the traditional academic boundaries, taking X-ray crystallography into chemistry, geology, biology, agriculture, materials science and medicine and much, much more.



John Jenkin, author of "William and Lawrence Bragg, Father and Son"

Lawrence Bragg rebuilt the physics departments at Manchester and Cambridge and rescued the Royal Institution in London, all against severe opposition, and history has judged him kindly in all three cases. He was surely one of the greatest scientists of the twentieth century. With his father he influenced a wider range of disciplines more profoundly than anyone else, and their achievements transformed our understanding of both the natural and the man-made worlds. He should be especially remembered and honoured on the centenary of his initial, pivotal discovery.

References

For further details of the Bragg story, see John Jenkin, *William and Lawrence Bragg, Father and Son* (Oxford University Press, Oxford, 2008hb, 2011pb).

For Lawrence, see Sir David Phillips, "William Lawrence Bragg, 1890-1971", *Biographical Memoirs of Fellows of the Royal Society,* 25, 1979, pp. 75-143.

The Braggs took science to the public, they supported schoolteachers and schoolchildren

The first five years

Margaret Elcombe

The formation of the Bragg Institute was the time when neutron scattering 'came-of-age' at ANSTO, no longer an add-on to the Materials or Physics Divisions. When formed, the Bragg Institute had two main teams, those involved with the HIFAR instruments (instrument scientists, technicians) and those involved in designing the first eight instruments for OPAL (lead scientists who got to go around the world to see what everyone else was doing and determine current 'World's best practice', engineers and draftsmen seconded from ANSTO Engineering) under the Head (Rob Robinson) and Technical Leader (Shane Kennedy). In typical fashion, the number of people outgrew the building (Building 58) very quickly, so a large annexe was assembled out the front to house them. When the Australian Synchrotron project staff joined us, even that was not enough and a second annexe was added out the back to accommodate them along with the increasing number of post-docs based with us.

Managing the transition from HIFAR to OPAL was well under way when the Bragg Institute was formed. There were five, soon to be seven operational instruments and all had recently been upgraded to ensure successful operation until HIFAR shut down. Some noisy detectors on the HRPD had been replaced (better quality data), a pneumatic shutter had been installed on the Medium-Resolution Powder Diffractometer (MRPD) (lower radiation dose to users), AUSANS had some new ancillary equipment (sample changer, Couette cell, sample temperature control) and improved software, LONGPOL had a supermirror polariser and 8 analysers and 2TanA had been given a motor upgrade with new driver software following irreparable failure of the old system. Two new instruments were ready to roll. The Triple-Axis Spectrometer (1970 vintage) had been converted to a strain scanner (TASS) to give the staff experience in residual-stress measurement and possibly encourage industrial users into the neutron field. An initially modest, but finally quite sophisticated, reflectometer had been constructed, some initial data had been collected and it was awaiting safety approval before commencing operation. It achieved five intensity decades of fringes from simple systems and allowed scientists to develop processing programs for the data. It was also planned to use it for testing supermirror guide sections during their production for the new era, although this did not actually happen: they were fully tested overseas.

Sample-environment equipment was adequate but becoming unreliable and difficult to maintain (lack of parts and expertise). New ancillaries were being purchased, but they had to comply with the new standards to allow them to be transferred to OPAL instruments. Where possible new techniques were being tested on the HIFAR instruments before being approved. Examples were:- the mounting for focussing monochromators for the powder instruments, trial of a small area detector for single-crystal data collection, the use of image plates and the testing of remote computer control of equipment on a simulated dance floor in B42. In anticipation of a much higher throughput of experiments, a computer-based scheduling system was already on line. Users could see the schedule from 'outside' and keeping track of who used which instrument for what proposal became a lot easier. The experience with this made evolution into the current database much smoother.

For four years the HIFAR instruments were run almost non-stop

The users were students, post docs, research scientists, whoever could get approval, getting as much data from the HIFAR instruments before the reactor was shut down. Students with theses to complete were given higher priority as we approached shut down.

In 2003 both TASS and the reflectometer received their first external users. Significant promotional activities were started (the new instruments were planned to be ~10x more powerful than the current ones). As a result there was a significant increase in demand from the Australian Institute of Nuclear Science and Engineering (AINSE) (proposals up 16%, usage up 28% and 14 new researchers), and ANSTO's Institute of Materials and Engineering Sciences was making good use of TASS. Availability of other instruments ~87%.

Construction of the Bragg Institute building

In 2004 a new instrument was commissioned. This was an X-ray reflectometer, to complement the neutron-reflectometer and was the first instrument operational in B82 (in an instrument cabin off the neutron guide hall). It was well used form the start. Neutron instrument availability was ~80%.

In 2005 there was a significant shift in emphasis to operations only (reduced technical effort) plus continued efforts to increase demand. Attempts to run LONGPOL at a shorter wavelength were aborted and it ran for the rest of its life at 3.6Å. Neutron instrument availability was ~90%.The 7 Tesla cryomagnet, received the previous year was finally commissioned both in the workshop and on the MRPD. A second X-ray instrument (SAXS) was commissioned in August and was also very busy from the start. Customer numbers and usage continued to increase. There was significantly greater use of the user feedback system and the ratings also improved. Users for OPAL were going to come from a much wider market than for HIFAR, which was still predominantly AINSE. To prepare for this change in users (adding ANSTO, ANSTO collaborators, and international researchers to the existing AINSE user base) a review system for the non-AINSE proposals commenced.

In 2006 activities started slowing down. LONGPOL ceased operation in March and 2TanA in June. The remaining instruments ran right up to the end. In April 2006, we found time to vacate Building 58, which had been the home to neutron scattering for ~35 years, and relocate to the new Bragg Institute building (B87). Laboratory facilities were relocated to OPAL's Neutron Guide Hall, with some user space temporarily located in B42, next to HIFAR.

The end of the HIFAR era came on January 30 2007, when the Minister for Education, Science and Training, Julie Bishop pressed the button to initiate HIFAR's final shut down.

In the 40 years I worked there, neutron scattering grew from four single-detector un-computerised instruments (data accumulated on rolls of paper tape and had to be taken to the site mainframe computer for processing) to seven highly sophisticated, computer controlled, instruments using single detectors, multidetectors or area detectors as appropriate, with an approximate 16-fold improvement in data-collection times.

There was also a nine-month decommissioning plan for all the neutron instruments inside HIFAR. As soon as practical after the shutdown, all re-useable items were removed from the HIFAR building and transferred into storage. 2TanA found a new home in the Powerhouse Museum in Sydney. Much later, months after the shutdown, when components had cooled down, I went back into HIFAR with the active handling crew and radiation survey worker to remove all the useable monochromators - large single crystals - from their shielding and transfer them across to storage in OPAL's Reactor Beam Hall. Some of them have since been used.

Ongoing throughout these years was the issue of licensing the new instruments with the Australian Radiation Protection and Nuclear Safety Agency (ARPANSA). At last, we had the chance to be our own master and not be licensed as part of the reactor. Preparing the submission to ARPANSA for this option (which involved going quite deeply into how the Australian Radiation Protection and Nuclear Safety (ARPANS) Act was framed) took a while, and getting approval took even longer. Having jumped that hurdle we then had to put it into practice, prepare documents for our operational practices, radiation safety, radioactive waste management and make sure the quality system for the Institute was up-to-date. While there was going to be a single licence for all the instruments, each one required its own set of documents and safety approval prior to cold commissioning. A new innovation (for us) was a Safety Interlock System to prevent personnel from being within any instrument enclosure when the beam was on. This was necessary because the thermal neutron fluxes were going to be an order of magnitude higher than in HIFAR and there would be general access to the Neutron Guide Hall. Initial ARPANSA approval was for hot commissioning only and operating approval was only granted once all the conditions had been met (predominantly that the radiation levels were acceptable). This two stage approval had not been envisaged originally. There are now two licenses, one for hot commissioning and a second for operation.

First access to the new buildings occurred in 2004. The new buildings were still 'under construction', so suddenly all staff with legitimate access needs had to have construction site licences and many of us dogging licences as well. The technicians needed access to set up the new workshop and the scientists to get ready for instrument components to arrive. We were even supplied with a controlled turnstile in the back fence to save the long walk round via the guard house. The first instruments installed there were not for neutrons but for X-rays, an X-ray Reflectometer (2004) and a Small Angle X-ray machine (2005). So even before the Neutron Guide Hall came into use designated room purposes were changed.

The contrast between the cramped conditions in the single HIFAR building containing the reactor and all seven neutron beam instruments and the huge warehouse-like initially empty Neutron Guide Hall at OPAL was staggering. At HIFAR, neutron scattering equipment was allocated 58 per cent of the main floor level along with an added mezzanine floor level for instrument control and storing sample-environment equipment. No longer was the instrument shielding design dictated by the ability to get it into position (AUSANS being the last and hardest to get in). The new instruments were designed for optimum performance including low radiation background levels.

Slowly OPAL's Neutron Guide Hall filled up. The guides were installed, with their shielding and monochromator shields, the dance floors laid, neutron instruments installed, much wiring done, computing control programs written and tested, Safety Interlock System installed and tested…. Everything you can think of for a single instrument times eight! A very busy time for all. So busy in fact that we could not get all the licences approved at the same time. There was some natural variation in the status of each instrument, dictated by the arrival of components. However to use the staff expertise as efficiently as possible it was also necessary to stagger actions round the instruments, completing an action (eg wiring, safety check) on one instrument before moving on to the next.

Eventually OPAL went critical (in August 2006) and finally produced sufficient neutrons for hot commissioning to start. Primary shutter open, radiation survey, secondary shutter open, radiation survey, instrument shutter open, radiation survey, increase power level and repeat – you get the picture. Slowly we worked up to full power. The first pattern was from ECHIDNA (in December 2006). Two months later (February 2007) we watched a full powder pattern from magnesium oxide build up on WOMBAT's computer screen in a couple of minutes. It was exciting. It worked. Then started the long haul of calibrations, detector efficiency calculations, aligning monochromators etc., before first publications were submitted to journals, later that year.

Installation of QUOKKA's vacuum vessel

Collaboration with colleagues in New Zealand on magnets and magnetism (2005)

Chief Scientist Penny Sackett, visiting in 2009, with Tony Irwin, Rob Robinson and Adi Paterson


Skating on Air, with AZ-Systèmes in Grenoble


Saurabh Kabra, Neeraj Sharma and Dehong Yu

ANBUG and the Bragg Institute

Chris Ling, Australian Neutron Beam Users Group

The Australian and New Zealand Neutron Beam Users Group (ANBUG) has always had a close working relationship with the Bragg Institute. Although ANBUG in some sense exists in opposition to Bragg, as an independent body representing the users with a duty to criticise (or praise) the facilities, the fortunes of the two have been intimately linked over the years. From its establishment in 1979 up until around 1993, ANBUG worked in a coordinated manner with the Physics Division of ANSTO to keep neutron science in the forefront of the scientific political arena. Acting as an independent body, it provided documentation to government agencies and review processes with a view to enhancing facilities at HIFAR. However, by the mid-90's, ANBUG was dwindling as HIFAR was falling increasingly far behind major overseas neutron facilities. The decision of the Australian Government in the late 1990s to fund OPAL and establish the Bragg Institute led directly to a revival of ANBUG's membership, in response to which a new ANBUG constitution was established in 2001. One of the first acts of this revived form of ANBUG was to successfully bid, together with the Bragg Institute, to host the International Conference on Neutron Scattering in Sydney in 2005. In the intervening period, corresponding to the design and construction phase of OPAL, ANBUG made many submissions to the project in direct support of the Bragg Institute and played an important role in its various Instrument Advisory Teams. Now that OPAL is fully operational, the relationship has returned to a more oppositional mode, but almost always to mutually benefit – happy users being more likely to return to the facility. A strong spirit of cooperation continues, exemplified in our recent successful joint bid to host the 2nd Asia-Oceania Conference on Neutron Scattering (AOCNS) in 2015, and we have no doubt that this will continue as ANBUG and the Bragg Institute grow in parallel.

Bragg Institute 10th anniversary

Oliver Kirstein, European Spallation Source, Lund, Sweden

Congratulations to all current and previous members of the Bragg Institute, established in 2002. Transforming a scientific construction project into an operating user facility that is amongst the leaders in the world is a tremendous achievement, and everyone who was part of the initial project, the transition period into and finally the operations phase should not only be congratulated but also proud of either having been or being part of something special.

Having the opportunity to reflect two years after leaving the Institute I experienced from its early beginnings until 2011, allowed me to recap what joining ANSTO Physics and the Neutron Beam Instruments Project in 2002 meant for me – in no particular order -

- Exciting opportunity to work in a different country…
- Fear of the unknown…
- How do I keep up some form of scientific work in parallel to running an instrument construction project…
- Growing together and becoming more than a team but rather some form of family…
- Experiencing people leave and colleagues grow…
- Proud of the opening ceremony when Prime Minister, John Howard inaugurated OPAL…
- Being one of only three instrument scientists who saw an instrument project like KOWARI go through all the phases from conceptual design up to commissioning and operations…
- Becoming one of the first staff members of the Bragg Institute…
- What will the future bring for me and my family in a foreign country…

It is a matter of life and growing up that one goes through different phases such as excitement, frustration, or even resignation at certain points. For me, being in the meantime responsible for my own group, the most valuable lesson I learned while being at the Bragg Institute was not so much related to running projects, but rather acknowledging the fact that the person offering a job takes as big a risk as the person taking it; I am grateful that I was trusted and that I had the opportunity to be part of an exciting journey. I hope that I will be able to apply what I learned while working with you at the Bragg Institute.

Recently, I had the opportunity to return to Australia and I was intrigued to see all the activities in the Neutron Guide Hall, the users on the different instruments and how the Institute has grown and transformed.

I am certain that the Bragg Institute will continue to be recognised for its activities in neutron scattering, and even more once the instruments that are currently being part of the NBI-2 project become available to the user community. I wish my colleagues all the best for the years to come, and I am looking forward to congratulating, and maybe even celebrating, the Bragg Institute's 20th anniversary in another ten years' time.

I am grateful that I was trusted and that I had the opportunity to be part of an exciting journey

Taiwan and the Bragg Institute

Rob Robinson and Wen-Hsien Li

One of the major successes of the Institute has been the involvement of the National Science Council of Taiwan (NSC) in the neutron beam program at OPAL, via its investment in the state-of-the-art cold-neutron 3-axis spectrometer, SIKA. Construction of SIKA was managed by the National Central University, under the leadership of Prof. Wen-Hsien Li, and user operations will commence in 2013, under the auspices of the National Synchrotron Radiation Research Centre in Hsinchu. At the time of writing in November 2012, SIKA has its commissioning licence and has received its first neutrons. Initially, it is using thermal neutrons, pending the return to service of OPAL's cold source.

The capital investment amounts to in excess of $8M, and the National Science Council is committed to placing four instrument scientists, along with one administrative assistant, and in return the Taiwan research community receives access to 70% of the beam time on the instrument, which may be spread over the full portfolio of neutron beam instruments at OPAL. In practice, the Taiwan research community is represented on the OPAL Program Advisory Committee, and participates in the normal user program, just like everyone else. Any discrepancies, and there haven't been many, are dealt with through Directors Discretionary time. The net result is that the Taiwan research community comprises the largest single overseas user community at OPAL, ahead of New Zealand and the United States, which are next.

The Taiwan involvement with the Institute results from plans to replace the Taiwan Research Reactor, which operated from 1973 to 1988, with the TRR-II Reactor. TRR-II was to be a 20-MW research reactor with cold source and an initial set of four instruments: powder diffraction, reflectometry, small-angle scattering and triple-axis, but the project was cancelled in August 2001. At that point, TRR-II's international advisory committee advised Taiwan to build an instrument at another neutron source in the Asia-Pacific region. Ultimately, this thinking led to the SIKA instrument at OPAL.

The first contact between ANSTO and these activities was when Rob Robinson was invited to attend a Workshop on Neutron and X-Ray Scattering: Applications to Biological and Industrial Problems in October 2001. Various other exchanges occurred thereafter, and a key player was Prof. Kuan-Ching Lee, who was seconded from the National Central University to the Taiwan Economic and Cultural Office in Canberra. The first Taiwan visit to ANSTO took place in early September 2003, and given that ANSTO was already committed to building high-performance versions of the four instruments envisaged for TRR-II, we converged on the idea of building a second 3-axis spectrometer using OPAL's cold neutrons. This was a sensible move for the whole facility, played to Taiwan's strengths and could easily be implemented on the CG-4 beam tube. The Chairman of NSC, Dr. Wei Che-Ho, visited ANSTO, including the OPAL construction site, in March 2004. This was followed up by another visit from Wen-Hsien Li and Kuan-Ching Lee in May 2004, at which the basic deal for the construction and operation of SIKA, and benefit to Taiwan users, was thrashed out. Of course this was very much in line with standard practice for such investments at neutron sources and synchrotrons around the world. Another year of negotiation, mainly over the particular use of words, resulted in a formal 'Arrangement' which was signed on 8th June 2005, and a subsidiary 'Services Agreement' between ANSTO and National Central University in March 2006.

The Taiwan research community comprises the largest single overseas user community at OPAL

With funding lined up, Peter Vorderwisch, who had recently retired from the Hahn-Meitner Institute in Berlin, after building and operating the FLEX instrument there, was engaged as a consultant and worked tirelessly at Lucas Heights for several years to assist in designing a state-of-the-art

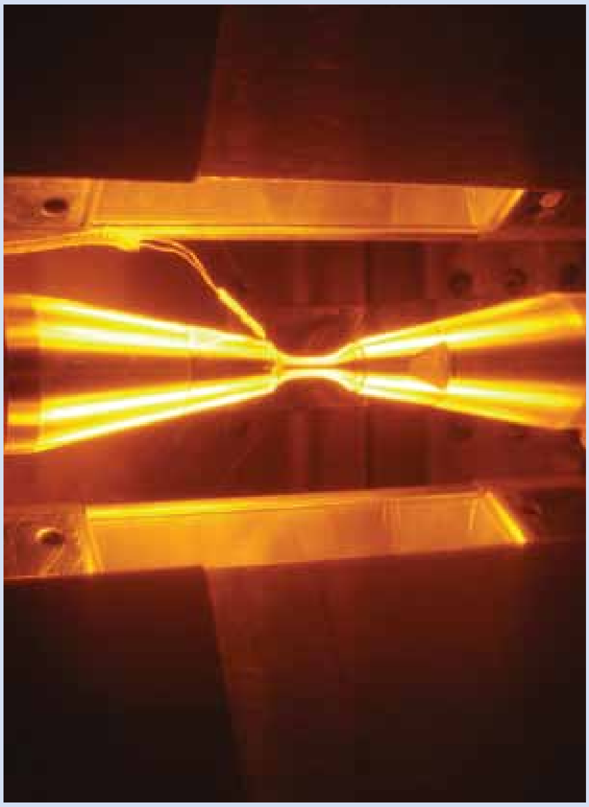
The Taiwan Connection

instrument. Charlie Wu did most of the work from the Taiwan side, and was assisted by Eno Imamovic, who was engaged to work on the design. The monochromators and drum were closely modelled on the adjacent TAIPAN thermal 3-axis spectrometer, but a much more complicated and versatile secondary spectrometer, modelled on BT-7 at NIST, has been implemented, together with a much larger dance floor. ANSTO has also contributed in the form of a ^{3}He polarisation system and cells for use on both SIKA and TAIPAN, and in the purchase of a 12-T vertical-field magnet and dilution refrigerator capable of reaching temperatures as low as 20mK.

In parallel, there were also significant interactions between Australia and Taiwan in the use of synchrotron radiation, particularly at the Taiwan Photon Source at Hsinchu. In preparation for the domestic synchrotron, the Australian Synchrotron Research Program installed a soft X-ray end station there, under the leadership and project management of Anton Stampfl in the Bragg Institute. With the commissioning of the Australian Synchrotron in Melbourne, the end station moved to Victoria and Anton moved to Lucas Heights, in order to join our triple-axis team on TAIPAN. But Australian collaboration with the National Synchrotron Radiation Research Centre continues strongly.

In summary, there has been a strong and growing collaboration between Australia and Taiwan, and particularly involving the Bragg institute, in the use of both neutrons and synchrotron X-rays, and this looks set to grow further in the coming decade.

Chris Ling president of ANBUG, awarding the ANBUG award for Neutron Science to Max Avdeev in 2011



High temperature Materials Science on KOWARI

Ordering Korean food at the first Asia-Oceania Conference on Neutron Scattering in 2011

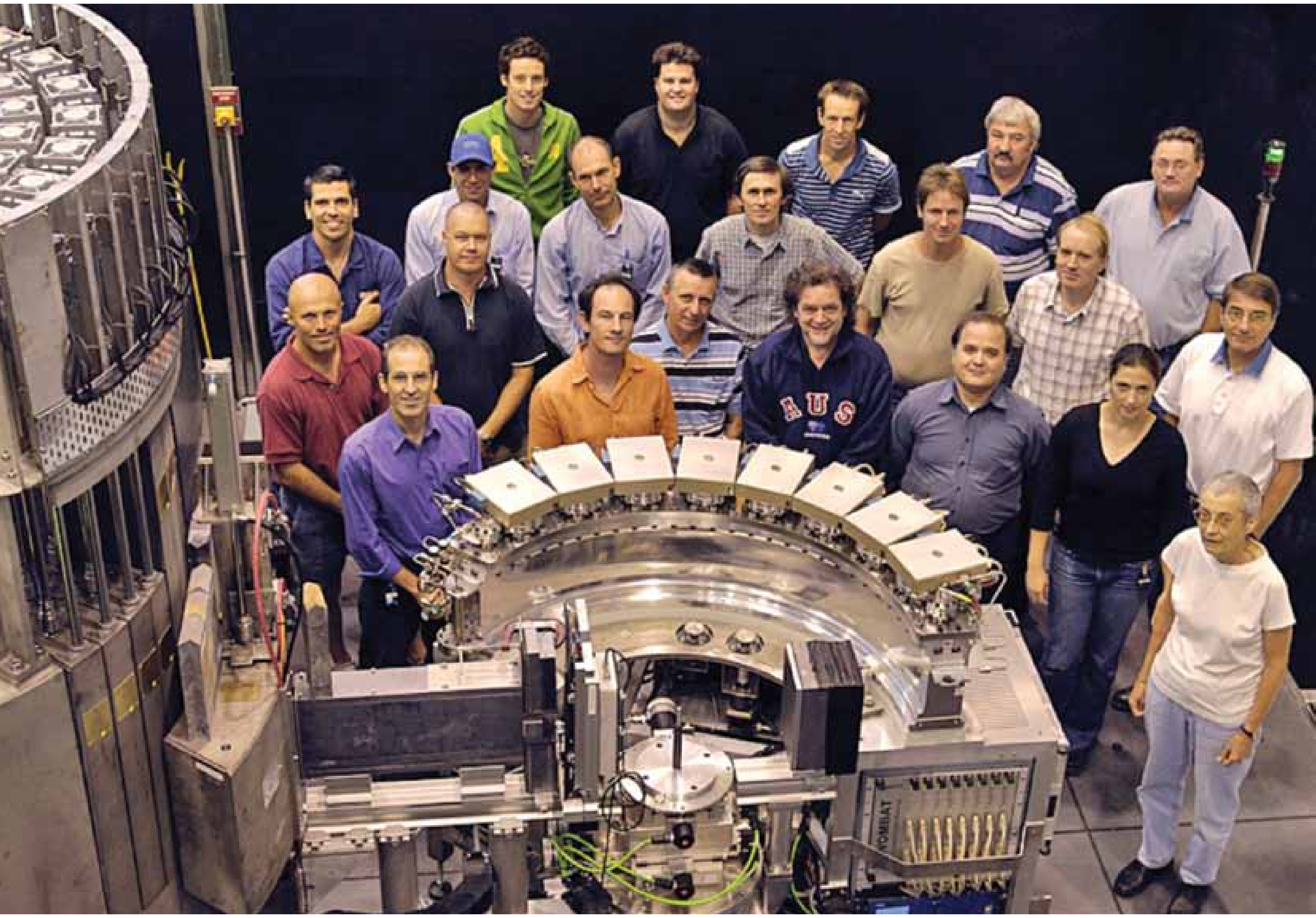
The ^{3}He polarisation station built for us by the Institut Laue-Langevin in Grenoble

Dan Bartlett and the PELICAN triple monochomator

Winning the Endeavour Award for Safety in 2007

Christmas with the Institute's children on the beach

Blue Mountains Workshop, December 2005



Many hands make WOMBAT: this photo, taken soon after ‘first neutrons’ with many of the people who contributed to its design and manufacture.

High speed neutron powder diffraction isn’t something that can be taken for granted

The world of WOMBAT

Andrew Studer

WOMBAT took its first diffraction pattern just after sunset on a day in early February 2007, a little less than five years after the beginning of the Bragg Institute. Margaret Elcombe, Vanessa Peterson and I watched the two dimensional diffraction pattern of magnesium oxide flash onto the screen seconds after having opened the beam. The MgO rod was a legacy of Margaret's sample collection from the HIFAR triple-axis instrument. It was a large sample used as a calibration standard. Even so, the quarter of a million counts per second we watched aggregating into the diffraction pattern impressed us all.

WOMBAT's ancestor was the Medium Resolution Powder Diffractometer (MRPD) at HIFAR. With MRPD, if you saw a pattern in 15 minutes you were lucky. Within days of WOMBAT becoming operational, we became impatient with any sample that didn't give a decent signal after 15 seconds. It was astonishingly easy to take the speed of one of the world's fastest reactor neutron powder diffractometers for granted.

High speed neutron powder diffraction isn't something that can be taken for granted. It's surprisingly rare. Some of the world's reactor facilities have only a single powder diffractometer, usually designed for high resolution in the tradition of Alan Hewat's design from the mid 1970's. OPAL's precedent was set at HIFAR with the two powder instruments there: when I arrived at ANSTO a few years BO (Before OPAL) there was MRPD, built by Shane Kennedy, and HRPD, built by Chris Howard and, at the time, operated by Brett Hunter.

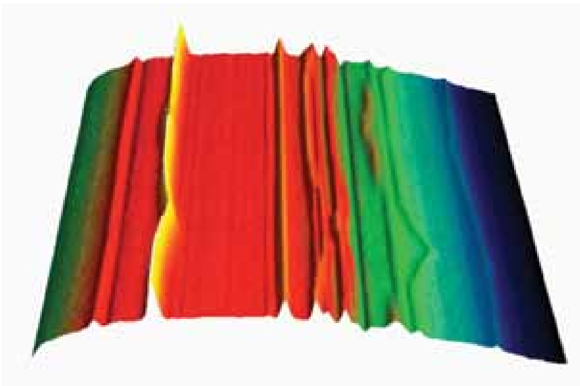
Powder diffraction was one of our strengths at the time, and so it wasn't a surprise that two powder instruments featured in Shane's earliest designs for the guide hall of the Replacement Research Reactor. But it was by no means a *fait accompli.* The plan survived the initial haggling over instrument priorities as a result of spirited and compelling representations from the Instrument Advisory Teams for ECHIDNA and WOMBAT. The legacy of Alan Hewat and Chris Howard meant that a high-resolution instrument was always on the cards, however it was the recent high-speed diffraction work of Erich Kisi's group done at the D20 instrument at the ILL that pointed towards the future. WOMBAT was to be a high-speed high-intensity instrument, with a diverse target audience looking at real-time processes and complex sample environments.

The building of the instrument really kicked off when Mark Hagen joined ANSTO. It was during his time that the instrument design came together and the most important procurement took place: the detector.

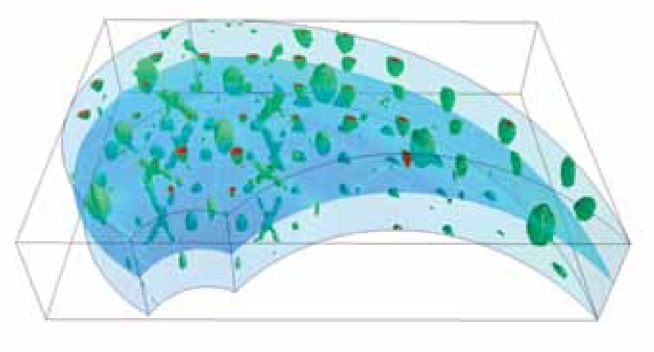
A world-class instrument needs world-class components, and for a high-speed instrument, the detector is crucial. Mark was responsible (along with many others at ANSTO) for procuring the curved 120° detector from the Instrumentation Division at Brookhaven National Laboratory, and after Mark left it was my privilege to visit Brookhaven periodically and see Neil Schaknowski, Joe Mead and the rest of Graham Smith's formidable team build and assemble a superb piece of neutron engineering.

At the Sydney end, under the watchful project management of Michael Deura and, later on, Shane Harrison, a band of technicians put together a superb beamline. It's unfair to highlight only a few, but I would mention Terry Noakes on design, Peter Baxter on integration and Mark New on fabrication for their vital contributions.

Since 'first neutrons' on that evening five and a half years ago, WOMBAT has proved itself to be a multidimensional instrument. We've done *in-situ* measurements examining batteries, clathrates and geological exchange reactions. We've looked at the high temperature performance of light metal alloys and the low temperature magnetic transitions in



An image of the first real-time experiment performed on WOMBAT: a lithium-ion battery discharge-charge cycle. This was a test experiment that yielded a beautiful dataset that was regularly used to show WOMBAT's power, especially during the OPAL shutdown of 2008. The data were later used as the basis for an article published as *Journal of Power Sources* 195, 8258-8266 (2010).



WOMBAT's role has broadened beyond its initial design specification for high-speed powder diffraction and now does experiments measuring texture, single crystal magnetism and diffuse scattering. This image shows diffuse scattering in a copper selenide single crystal.

intermetallics. We've done high speed stroboscopic measurements of electroceramics. We've looked at Bragg and diffuse scattering from several single-crystal systems and done a dash of pair-distribution function analysis. We've gassed, squished, frozen, melted, heated, spun and magnetised. We've run about twenty different sample environments on WOMBAT, and in the near future will add polarisation to its capabilities. WOMBAT has proven to be a far broader instrument with a more diverse user base than originally foreseen.

Friedl Bartsch and Andrew Studer in front of the WOMBAT detector

Laue Diffraction on KOALA

Alison Edwards

The 1912 report of the diffraction of X-rays by crystals occurred when both radiation and atoms were less well understood than at present. Indeed the report of diffraction of X-rays by a crystal was a fundamental proof of their wave-like properties. The interpretation of these diffraction images by Lawrence Bragg in terms of a set of atomic sites which when combined with symmetry operators comprise a 'crystal structure' proved the greatest single advance for chemistry in the 20th century.

KOALA, the Laue diffractometer implemented at OPAL provides for single-crystal neutron diffraction experiments capable of filling in many of the blanks which X-ray diffraction, being due to electron density, could not. Hydrogen – the smallest element – is particularly ill-defined by X-ray diffraction, so many aspects of the chemistry of hydrogen remain to be

KOALA and Ross Piltz

KOALA and Alison Edwards

defined within the structure-reactivity paradigm at the heart of modern chemistry. The incomplete understanding of hydrogen, in all its chemical combinations, is a significant gap in fundamental knowledge with important implications in many proposed commercial and industrial applications. Whilst having far broader application, the Koala diffractometer is now established as the instrument of choice for chemists seeking full understanding of the presence and potential reactivity of hydrogen in the compounds they seek to understand.

Hydrides in potential catalyst materials:

Hydride, H^-, is frequently found in compounds prepared as potential catalysts or catalyst models for industrial chemical processes. Verifying absence or presence of hydride, and defining its structural properties when present, remain a challenge for workers in this area where Australia has several high-profile groups. A collaboration with a major group at RIKEN, in Japan, is also underway.

Understanding the possibilities of hydride:

Hydride is the smallest atomic anion and the prospect that it could be a key component in energy storage applications is well recognised. The absence of a sufficient data base of reliable structures from which a systematic understanding of hydride can be derived is a major deficit in attempts at rational process design. Collaboration with a Taiwanese group has to date demonstrated two new coordination modes for hydride and proved the presence of hydride in compounds where it is only a fraction of a per cent of the weight of the material yet is a key element in the material's behaviour.

Understanding the hydrogen bond:

Hydrogen bonding is a strong force in intermolecular terms, but frequently, hydrogen positions and conclusions based on them are inferred from inherently inadequate X-ray data. Collaborations have been established in Australia, the UK and India which address this issue at a range of levels – from determining whether a hydrogen nucleus is located on one or another site where electron density is found (but where a pair of electrons may exist without forming a bond) through to detailed high-resolution mapping of electron density in X-ray studies by comparison with neutron diffraction derived nuclear site definition to prove whether an evident short contact between two atoms is accompanied by an electronic (bonding) interaction.

Ten years of sample environments at the Bragg Institute

Paolo Imperia, Scott Olsen and Stewart Pullen

Sample environment is fundamental for a properly run user facility

It is not often that neutron scattering experiments are performed under normal ambient conditions. Since the early days it was clear: to successfully run a user oriented facility at the same level as the best institutions worldwide, beside a suite of world-class neutron instruments, a good mix of equipment for sample environment is also necessary.

Sample environment provides the equipment necessary to run experiments at very low or very high temperatures, under high gas or mechanical pressure, under a high magnetic field, a voltage or under a combination of the above or more. The sample environment group also provides solutions for specific experiments, for example, neutron scattering experiments done simultaneously with other techniques: optical techniques, gas sorption experiments etc...

Early days

Prior to the Bragg Institute forming, there was a small suite of sample environment equipment for use on the HIFAR instruments. This included a top-loading cryocooler and a bottom loading one, Eulerian cradles and 2 furnaces made in house by Merv Perry, the first technician dedicated to Sample Environment and working on this equipment since 1991. Of these, one Eulerian cradle, one bottom-loading cryofurnace and one in-house-built furnace are still in use today.

Neutrons are particularly apt for research aimed at magnetic materials. It is not surprising then that the first purchase (in 2005) by the Bragg Institute was a 7-Tesla dry vertical-field cryomagnet funded via an Australian Research Council grant with substantial university co-investment, which is still in use today. It was one of the first cryogen-free (or ‘dry’) magnets, an innovative piece of equipment that has been extensively used despite its shortcomings: a small window, designed for HIFAR necessities, and high background.

When the Neutron Beam Instruments project started in 2000, there was A$750,000 allocated for sample environment equipment. This was used to purchase an ILL-type 1700°C vacuum furnace, an ILL-type liquid-helium ‘orange cryostat’, and new bottom-loading cryofurnaces, one of which was dedicated to the 7T vertical magnet.

Once the OPAL reactor started in 2006, a significant amount of extra funding (A$2 million) was made available to purchase a large range of sample-environment equipment for hard condensed matter including a 5T high-temperature superconducting horizontal-field magnet (2007) in partnership with New Zealand, a 100kN horizontal load frame for the strain scanner (2008) with a furnace design copied from ISIS. A 1T Electromagnet and cryocooler, and an 11T wet horizontal cryomagnet with ^{3}He one-shot fridge (2009) and optical windows for SANS experiments. Later two top-loading cryofurnaces arrived, allowing a much easier and faster sample change, along with a ‘Cobra’ single-crystal sample cooler for KOALA. Finally, based on user feedback, a dry toploading cryocooler for the 7T vertical magnet capable of 1.5K was purchased in 2011. For soft condensed matter, a range of equipment was also purchased including Langmuir troughs, a Differential Scanning Calorimeter, an impedence spectrometer, numerous solid-liquid cells, stopped-flow cells and a rheometer. For high pressure work, a Paris – Edinburgh cell was commissioned with the ability to apply pressure to samples up to 10 GPa.

In 2009, a further injection of capital to sample environment, with the Neutron Beam Expansion Program (NBI-2), allowed us to design and procure a new suite of high-end equipment. In 2012 a new 12T vertical-field magnet has been commissioned. The design was done keeping in mind the necessities of the 3-axis instruments, TAIPAN and SIKA, and the PELICAN time-of-flight instrument and the need to do polarisation analysis on all instruments. The magnet has a sample rotation stage, and a 340 degree scattering angle. Single crystal mapping is possible with this magnet. The magnet is a classical wet magnet with a He recondensing stage. It needs a very modest amount of liquid He re-filling to keep it cold.

Gene Davidson transferring liquid nitrogen with QUOKKA in the background

The 12T magnet was procured together with a 20 milliKelvin dilution refrigerator insert. This combination will allow cutting-edge research on exotic states of matter like Dirac strings, spin-ice states and so on.

Further procurement, within the scope of the NBI-2 program, included a new sorption system for *in-situ* absorption and desorption measurements, with five gas streams allowing controlled mixtures of gases up to 200 bar, a vapour delivery system and a large amount of basic equipment like turbo-molecular vacuum pumps, roughing pumps and the everyday minutiae like tubing, cabling and all the related and associated electronics and controllers necessary to deliver excellence to a growing facility.

In-house design of equipment.

The in-house development of specialised sample environment equipment has provided a great capability to the Institute over the years: from the development of air furnaces to vacuum furnaces, pressure cells ranging from 100 to 3,500bar and special one-off equipment like the 'Rapid Heat and Quench Cell', the Environmental Chamber, Rapid Sample Quencher and most recently, an *in-situ* Differential Scanning Calorimeter for SANS. All have allowed the Institute's Scientists and the user community to conduct their experiments under the conditions that off-the-shelf products cannot deliver.

The most important feature of this group is its adaptability, with an ability to respond rapidly to the needs of the research community

Ten years of sample environments at the Bragg Institute

Paolo Imperia, Scott Olsen and Stewart Pullen

The group has delivered engineering solutions to complex problems, some being recognised by Engineers Australia through their Excellence Award program. In addition to our development of various pieces of sample-environment equipment, we have made numerous interface designs that allow various sample mounts and geometries to be used within our suite of equipment. This has often allowed highly successful experiments that would otherwise not have occurred.

The most important feature of this group is its adaptability, with an ability to respond rapidly to the needs of the research community, something that is of great importance, and which will continue to contribute to the Institute's success .

Temperature range

During the HIFAR days, our dry cryocoolers could operate in the range from 5K to 300K. The minimum temperature range was extended to reach 1.5K in 2007, with a wet cryostat, 0.4K in 2009 with a ^{3}He refrigerator and finally 0.02K with a dilution refrigerator in 2012.

Thanks to the inventiveness of the Sample-Environment team, this 'standard' temperature range has also been extended upwards with the standard cryostats up to 800K, using special purpose-built high-temperature sample holders. These allow a full temperature range from 4K up to 800K with a single cryorefurnace.

In the HIFAR days, an air furnace capable of heating the samples up to 1100°C was built by Merv Perry. This furnace has recently been refurbished and is used occasionally on WOMBAT and ECHIDNA. It has a high background and small window, but is a robust and reliable piece of equipment. The current maximum sample temperature today is 1700°C using the ILL vacuum furnace purchased in 2006.

Growing users support, continuous improvement

The sample-environment group has been established from the beginning to take care of the equipment, and to deliver a problem-free experience to the scientific community, with a goal of smoothly running complex experiments requiring special environments. In this way, when the technical problems are minimised, the instrument scientists can fully concentrate on the scientific side of the experiments; the data analysis flows and papers are written. The first appointed manager of the Sample Environment group was Scott Olsen in 2006. An engineer by trade, he developed the group and started the international cooperation with other groups around the world. In 2009 Paolo Imperia took over the responsibility of the major capital projects and in 2011 has been appointed as successor of Scott as a group leader with operational responsibility. In 2010 the Bragg Institute's international standing in sample environments was recognised with the award of the hosting rights for the 7th International Sample Environment workshop held in Sydney in September 2012.

Our people

Scott Olsen, Sample-Environment group leader 2006 to 2011

Paolo Imperia, Sample-Environment group leader since 2011

Merv Perry, started as unique sample-environment specialist at HIFAR

Gene Davidson, dedicated specialist to cryogenics and magnets since 2005.

Norman Booth, recently joined the group to take care of sorption, equipment for soft-matter and high-voltage experiments

Stewart Pullen, started as an honours student in engineering with University of Western Sydney, and has designed and managed the projects for the construction of the purpose-built sample-environment equipment

Students

We have hosted a constant stream of summer students and year-in-industry students. These students have delivered excellent results on our *ad-hoc* projects and several of them, after the experience in the Sample Environment group, have continued to do research with neutrons.

The engineering team

A support team of mechanical technicians has also assisted the sample environment group, since the OPAL reactor started: Marty Jones, Andrew McGregor, Mark New, Matt Bell and Tai Nguyen.

A group of design mechanical engineers was formed at the end of 2010 and they often assist with design and approvals: Stewart Pullen, Steven Pangelis, Jim Palmer and Adrian Ogrin.

A Gumtree retrospective

Nick Hauser

What is Gumtree?

Gumtree is a graphical user interface for instrument control, data acquisition and data reduction.

Why was Gumtree created?

In 2002, Elliot Gilbert (QUOKKA instrument scientist) explicitly requested a graphical user interface for the instrument he was building and allocated budget towards its development. Other instrument scientists required only a command line interface and provided minimal budget.

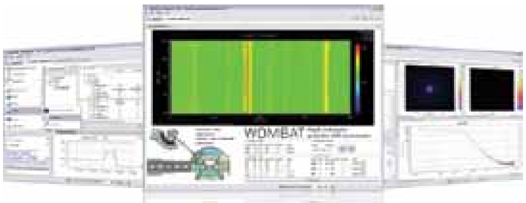
A workshop held in December 2002 confirmed Elliot's request for a graphical user interface (GUI). The user community requested a GUI to make it easier for users to operate an instrument without remembering text commands and syntax.

At that time, there were no 'out of the box' solutions. Solutions were available for device servers, but no one had provided a framework that could be easily configured to control an instrument with a GUI. This situation has changed significantly in the last 10 years and now there are several open-source solutions that have been developed by the neutron and X-ray scattering and accelerator physics communities.

A difficult decision was made in early 2003 regarding instrument control. The Paul Scherrer Institute (PSI), in Switzerland, had a minimalist but robust instrument control application with a command line interface, known as SICS (SINQ Instrument Control Server). It had no graphical interface and it wasn't going to be straightforward to build one. However, we knew that we could get the instruments running with the least amount of resource and risk using the PSI solution. It was decided to use SICS. This decision transferred risk and resources into the graphical user interface development.

Who created Gumtree and where?

Andy Goetz spent 2003 with the Bragg Institute on sabbatical from ESRF Grenoble, and is credited as the creator of Gumtree. Andy loved the Australian bush, especially the outback. Since the instruments



were given Australian fauna names, it seemed appropriate to call the control application Gumtree, that ubiquitous, tough Aussie eucalypt. Andy played a leading role in the creation of Gumtree, and the recruitment of Tony Lam, Gumtree's lead developer. Andy is a prolific software inventor, having created products including the TANGO device server and the FABLE / DAWN visualisation applications. Andy had 17 years' experience with ESRF at the time of Gumtree's creation.

Why Java and Eclipse?

It was a requirement set by instrument users that the application be cross-platform, explicitly Mac, Linux and Windows, so that instrument users could install Gumtree on their favourite operating system. Hence Java was the chosen language. However, it came with a compromise; the range of scientific applications was limited, especially plotting and data manipulation. These applications would appear in the open-source in later years, but caused major challenges early in the project.

The choice of the Eclipse Rich Client Platform (RCP) provided benefits and additional constraints to those of Java. The major benefits were Eclipse's plug-in architecture, which promised simple integration of third party plug-ins to enhance Gumtree's features. The second benefit was Eclipse's windowing environment, which controlled the many views required for instrument control, data acquisition and data reduction that are required for the many techniques that Gumtree was commissioned to facilitate. Eclipse RCP was first released in the year that we started using it. Lesson 1: Never use bleeding edge technology. The constraint was that RCP had no scientific plugins at the time and it used a graphical technology called SWT, which would further reduce our options. Yes, we were painted into a corner and were waiting for the paint to dry. As with all computer languages and frameworks, there was a long and steep learning curve. In addition, RCP had new software engineering concepts which were difficult to understand. From 2004 to 2008 the door to the development team's room was revolving, with 13 developers coming and going through that period, with an average stay of just over a year, only long enough to learn the technology. Two developers stayed for more than three years and have made the most significant advances in Gumtree. By comparison, the SICS application has four developers since 2004, the lead developer since project initiation.

It was difficult to define a protocol to connect Gumtree to SICS. A breakthrough was made by our PSI collaborator, Mark Koennecke, with his invention of the hipadaba (hierarchical database) interface to SICS, and Ferdi Franceschini and Tony Lam using the json protocol to encode messages. This allowed SICS to have an interface that was machine friendly.

In hindsight Gumtree would have been done differently. It would have been simpler and used more conservative technology. It probably should have been developed to run on a single operating system and as a single application, rather than using the client-server pattern. If the project had started in 2008, the 'Generic Data Acquisition' from the Diamond Light Source or the 'Control System Studio' from Argonne and DESY would have fulfilled the user requirements. Interestingly, both these products are built on the same Eclipse RCP platform.

Does Gumtree work?

All the challenges were overcome and Gumtree is now operating on five of the seven operational instruments.

The key to getting Gumtree to work has been to tame the complexity of the Eclipse beast by creating simple components. This sounds easy, but in practice was difficult. Now the beast is tame, and effort is being put into the Gumtree's original purpose, to make running neutron scattering experiments easy for novice users. We're not there yet, but we believe that we're on the right track.

This sounds easy, but in practice was difficult

Has anyone else adopted Gumtree?

The SINQ at PSI created a minimalist version of Gumtree (known as Gumtree Swiss Edition). The Soleil (France) and DESY (Germany) synchrotrons collaborate with ANSTO over Gumtree's data object plugin (CDMA).

What is the future?

It is a vision for the future that there be a best-of-breed solution for instrument control for the X-ray and neutron scattering communities which is a collaboration of many facilities. With the Bragg Institute working more closely with the Australian Synchrotron, it would be beneficial in the short term for both organisations to adopt a common solution.

Acknowledgements and thanks

Bragg Institute instrument scientists for ideas, feedback and support.

Andy Goetz, Mark Koennecke, Tony Lam and Norman Xiong, the creators and problem solvers.

Paul Hathaway, Andrew Campbell (year in industry), Hugh Rayner (year in industry), Ziwen Liu (year in industry) Adrian Chong (vacation), Darren Kelly, Bernadette Garner, Jian Gui Wang, Lindsay Winkler, Danil Klimintov, Rodney Davies, Lidia Zhang, the developers.

Rob Robinson and Shane Kennedy for sponsorship and support.

Motofit

Andrew Nelson

Arrival of PLATYPUS's vacuum vessel in 2006

The technique of neutron reflectometry has become very popular in the past few decades. This is because it is adept at studying the structures of thin films at interfaces, such as the polymer films found in organo-photo voltaics, or the interaction of proteins with bilayer membranes. The rapid expansion of the neutron reflectometry community has been aided, in part, by the development of advanced reflectometers, SURF and INTER at ISIS, FIGARO and D17 at the ILL and PLATYPUS at OPAL, to name but a few. These reflectometers have pushed back the frontiers of the technique, with the complexity of experiments increasing rapidly. Consequently, the volume of data streaming from these instruments has expanded greatly, but in many cases the scientists obtaining the data have not been able to keep up. This is mainly due to the lack of analysis tools available to the community that scientists can master and that are advanced enough to cope with the wide range of datasets thrown at them.

The Motofit program started development in 2005 to address these issues. Its initial focus was the ability to do least-squares co-refinement of multiple contrast (X-ray and neutron) datasets within an easy to use Graphical User Interface (GUI) based program. Multiple contrast co-refinement helps alleviate the phase problem, allowing unique structures to be identified. Whilst programs with this ability already existed, they were hard to use and were not within easy reach of the average scientist. Unfortunately the GUI based analysis programs available at that time could not co-refine multiple datasets. Motofit immediately solved that issue, marrying advanced functionality and ease of use in a single program.

Since its initial conception, development has been continuous, making several cutting-edge advancements available to the reflectometry community. Two examples are:

- genetic optimisation – essential for global optimisation of multi-variable least-squares systems.
- batch fitting – kinetic measurements produce hundreds of datasets which need to be analysed in a consistent manner, without taking a long time.

The utility of the Motofit program has meant that it is now one of the most popular programs of its type around the world, with around 150 citations since its inception (30 citations/year). Its popularity has led to new scientific collaborations between myself and researchers from around the world. These collaborations have advanced new features in Motofit, such as the application of Chebyshev basis sets and cubic – B – splines in freeform modelling approaches, as well as attracting new users to the PLATYPUS instrument.


Showing Senator Chris Evans around in 2012

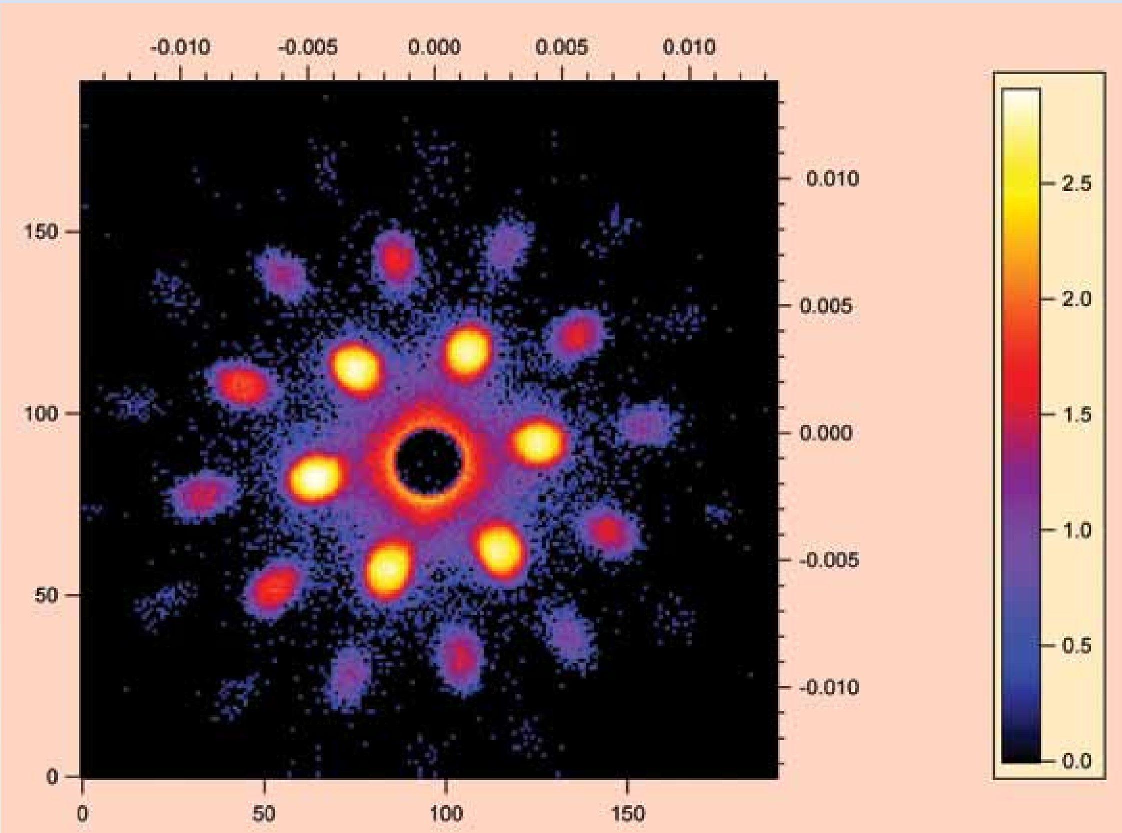

The Beam Instruments Advisory Group in 2003


Dino Ius and our all-digital safety interlock system


A leaving party in Bangor in 2009


Showing Cardinal George Pell around in 2006

The Bragg Institute in 2007



Small-angle scattering from the superconducting flux-line lattice in niobium on QUOKKA

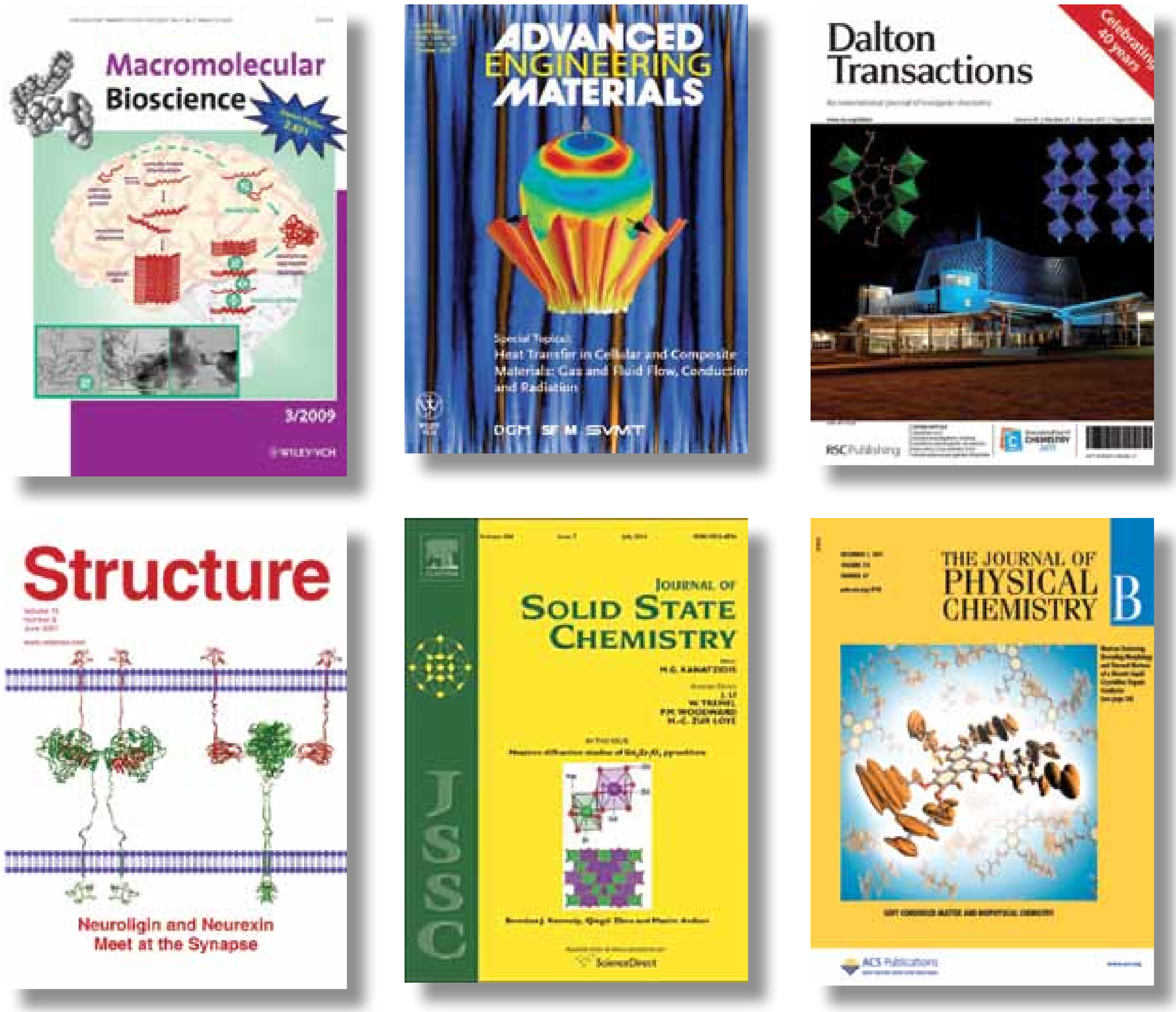
The characterisation of biomolecules project and the birth of the National Deuteration Facility

Peter Holden

In the year 2000, I was a member of a small team of biologists/microbiologists/biochemists in ANSTO's Environment Division. At that time, it had become apparent that our strategic position and relevance to ANSTO's research effort was increasingly becoming marginalised, in part because of a move away from the study of mine-site impacts and in part because of the Executive's view that we lacked critical mass and weren't essential. Personally, a key symptom was that 60 per cent of my time had been diverted onto working on development and certification of ANSTO's Environmental Management System which in reality consumed much more time. In the face of this, I began contemplating how to re-orient us to ANSTO core business and the obvious question was how we could involve ourselves with science related to the new OPAL reactor which was under construction. From these musings began a somewhat misguided search for information on neutrons. I thought I had heard of neutron microscopes and a senior environment manager indicated vaguely that he believed the Russians were doing such work. I hadn't heard about the Bragg Institute and really knew nothing about what had been done at HIFAR previously. Coincidentally, ANSTO had an externally designed corporate learning initiative (LENS) in play, which emphasised active learning and required staff to undertake ALES (Active Learning Exercises – not Fosters!) in teams and the biologists banded together to do one on neutron scattering. We searched the literature and had some early interactions with Bragg Institute staff, including Robert Knott and Mike James.

Early in 2001, I had discussions with the Director of the Environment Division, Professor Ann Henderson-Sellers, about the desire to put forward a new project and the suggestion that it be on biological applications of neutron and X-ray scattering. She encouraged me to do so and I also began to have some interaction with Rob Robinson who was responsible for the Bragg Institute. At that time, Robert Knott was the only person in the Neutron Scattering and Synchrotron Radiation Group who had extensive experience in biological applications of scattering (SANS for structural biology) and the Environment team were the only research biologists at ANSTO and so we thought that we were well placed to drive the proposal forward (ignorance is bliss). ANSTO had a process for new projects which of course involved a relevant form (the Project Definition form F 7.2-001). The vetting process included internal presentation to Environment's Director and management, presentation to the relevant ANSTO Core Business Area Committee, presentation to the ANSTO Executive, and if still surviving, a final step involving presentation to ANSTO's external Technical Advisory Committee in March 2002.

The 'Characterisation of Biomolecules' project (Biomolecules) survived these various steps although it suffered a reduction in scope and staff resources along the way. The project officially started in July 2002 as a 12-month Scoping Project and had a resource of slightly more than four person-years, made up of small slices of a number of people and larger portions of biological effort. The initial emphases of the project were on environmental issues and biomaterials (particularly biopolymers) which reflected the expertise available at the time. People involved in the early stages included Kerie Hammerton (haemoglobin biochemistry), John Ferris (diatom structure), Peter Holden, Rob Russell and Karyn Wilde (biopolymers in collaboration with John Foster from UNSW), Chris Garvey (cellulose, haemoglobin, red blood cells) who was recruited as a post-doc in November 2002 after having completed part of a term with Robert Knott and having gained some SANS experience, John Bartlett (Materials Division – Sol Gel chemistry) and Ned Blagojevic (Biomineralisation). We also nominally had 10 per cent (at various stages) of Robert Knott's, Mike James's, Elliot Gilbert's and Jamie Schulz's time although initially it was difficult to squeeze out time away from the Neutron Beam Instruments project. Robert had an involvement with supervision of a PhD student Lisa Rodgers who investigated immobilisation of an enzyme in sol gels using SANS (co-supervised by John Bartlett, John Foster and myself). In 2004, Biomolecules jointly funded a Post Doc together with Mike James and Hans Coster (University of Sydney) to provide some resource to devote to neutron reflectometry on biosensors and this led to a long and enduring involvement from Mike James who made the push into biosensor and biomembrane work



A selection of magazine covers with articles from the Institute

succeed. We have had a succession of bright young post-docs who provided the effort and mental grunt to do this work – including Alicia Wong, Bee Gan, Hanna Wacklin and Anton Le Brun. We have also benefited from Andrew Whitten, Cy Jeffries and Augustine Yun's efforts in the areas of structural biology and polymers.

During the initial genesis of the Biomolecules project, I attended a Workshop on Neutrons in Biology held in Melbourne in July 2001 which was to have a lasting effect on my thinking about strategic directions for the project. I distinctly remember Jill Trewhella stating that molecular deuteration was the key to advancing biological applications of scattering (or at least SANS). Helpfully (and not surprisingly) the workshop report had two key recommendations that I used to help justify the project:

- the small-angle neutron scattering and reflectometry instruments in the RRR be pursued with high priority
- a small number of regional facilities be established (or enhanced) to allow users to perform deuteration of biomolecules. These facilities would be of significant value to the NMR and neutron scattering communities.

The former confirmed my focus on these techniques but in the latter I saw an opportunity to carve a niche – one that would call on the microbiological expertise possessed by Holden, Russell and Wilde.

Our initial foray in this area was to produce deuterated biopolyesters of the Poly-Hydroxyalkanoate (PHA) class. These are carbon/energy storage bodies produced by bacteria when carbon is present in excess and other nutrients are limiting. John Foster (UNSW), one of my previous collaborators, was an expert in these biopolymers and I proposed that he should get involved. In 2004 we produced several PHAs that varied in degree of deuteration. External reviews of the project by John White and Peter Timmins strongly supported biodeuteration as 'essential' and development of this capability was adopted as a high priority.

In 2005, I lobbied the Executive to fund an expansion of Biomolecules capability development to include protein chemistry, indicating that for SANS applications, the majority of bioscience would be for the Structural Biology community and would require in-house facilities and expertise. By early 2006, Agata Rekas and Anthony Duff had started and they began the process of establishing a protein lab including the equipment to enable purification and chromatographic separation of proteins produced using expression of cloned genes in bacteria.

Thus, we entered 2006 with capability development rolling on for biodeuteration and Structural Biology using neutrons when “manna from heaven” dropped on us in the form of the National Collaborative Research Infrastructure Strategy (NCRIS), a federally funded scheme to establish major national research infrastructure. The NCRIS Road Map, the guide to funding submissions and the selection process, clearly stated that with the new neutron beam instruments about to come on-line at OPAL, “the most immediate priority … is the provision of a deuteration facility”. With the Biomolecules project and its initial demonstration of biodeuteration of biopolymers, ANSTO had no competitors seeking to provide this facility using NCRIS funding and the strategic decision to pursue deuteration and protein chemistry for structural biology bore fruit. The NCRIS submission process also led to a substantial forward commitment to deuteration activity on ANSTO’s part.

In November 2006, $3.3 million in NCRIS funding was announced and the National Deuteration Facility (NDF) was born. NCRIS and ANSTO funding enabled us to expand our bioreactor capacity, employ a full time molecular biologist (Vanessa Lake) to undertake the required cloning of genes for expression of proteins, and to acquire a suite of instruments to characterise the biomolecules we deuterated – both proteins and polymers. Marie Gillon also joined the team to provide technical support. The NCRIS funding also provided the impetus and funding to establish Chemical Deuteration of small organic molecules – achieved by catalytic exchange and synthesis. The team of Paramjit Bansal, Tamim Darwish, Emily Luks and Greta Moraes was recruited, new labs were created by refurbishment of office space in B22 and key instruments such as a 400 MHz NMR and an LC:MS/MS were procured and commissioned. The activity of the Chemical Deuteration team is described elsewhere in this book.

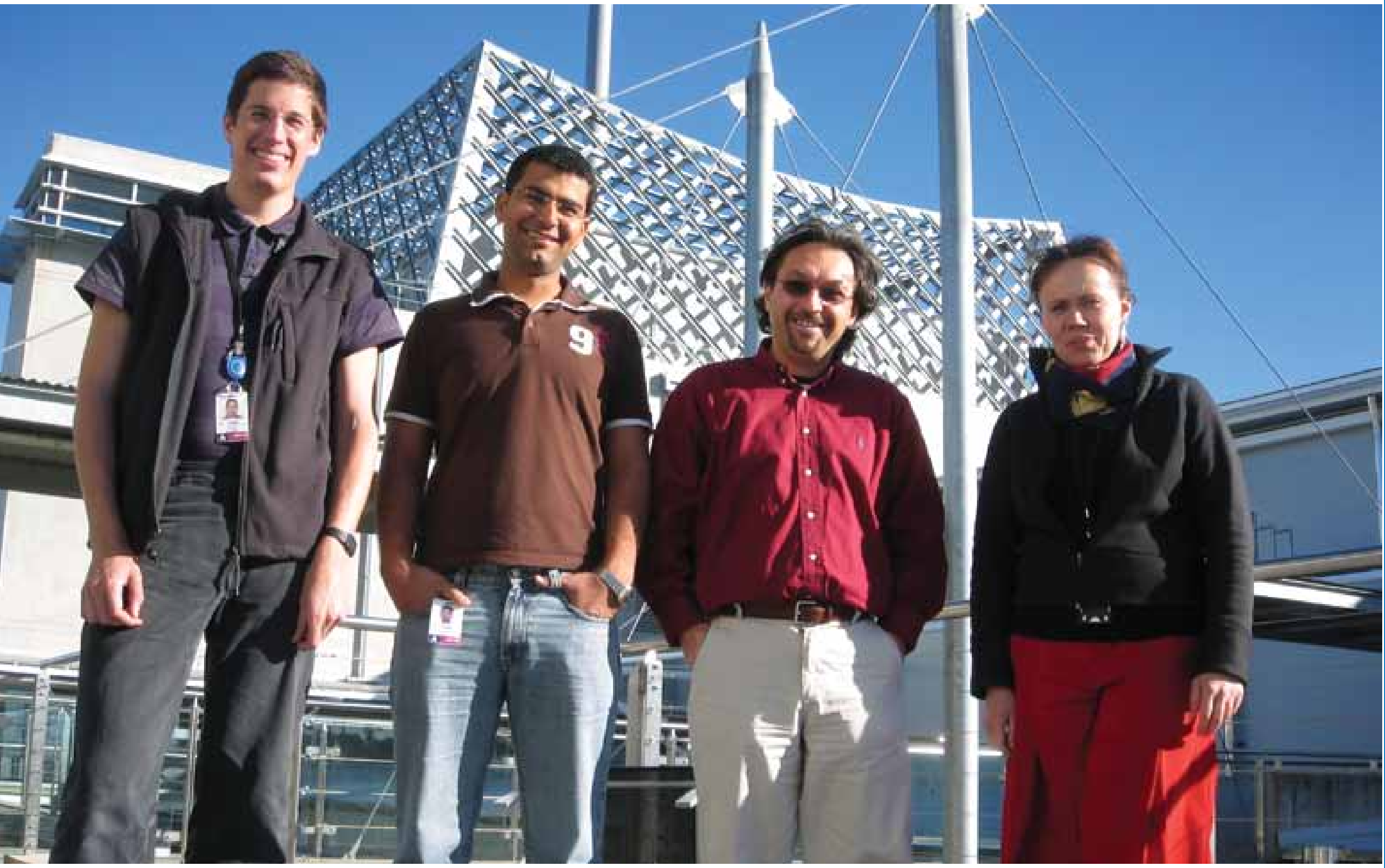
In 2008, the NDF left the Institute for Environmental Research and became a stand-alone research unit and in 2009 it merged with the Bragg Institute to build a closer connection between staff undertaking the neutron beam instrument user program and the NDF staff. In mid-2009, we had the first call for proposals through the Bragg Institute User Portal for biodeuteration of molecules (principally proteins and polymers) and at the end of the year the second call included Chemical Deuteration for organic molecules. Since that time we have been oversubscribed for deuteration proposals, although current issues with cold-neutron availability have tempered the initial burgeoning of demand. In 2012, Paramjit Bansal and Emily Luks left the NDF and we were joined by Rao Yepuri – a synthetic chemist.

Molecular deuteration was the key to advancing biological applications of scattering

The NDF has now deuterated approximately 120 molecules and in the last 12 months or so we have seen the first high-impact journal papers showcasing applications undertaken at OPAL using these molecules. The range of applications has included both cold and thermal neutron techniques. We have also produced labelled molecules for structural investigations using NMR ($^{2}H/^{15}N/^{13}C$ labelled proteins) and Synchrotron-IR (d-PHAs). It is worth noting that the Biomolecules/NDF effort has now passed the 100th published paper mark. None of this would have been possible without the dedication of the staff, or without the involvement of many external collaborators as from the outset we sought to develop our capabilities by partnering with university sector researchers to explore real problems. We look forward to more exciting science in the future.

Food Science

Elliot Gilbert



The food science team circa 2009: Jaroslav Blazek, Jitendra Mata, Elliot Gilbert and Anna Sokolova

The Food Structure and Dynamics project, commonly known as Food Science, started formally in 2005 but pre-dates this by three years when it was informally proposed by Stuart Carr, former head of ARI. Rob Robinson approached me in 2004 and suggested that I might wish to propose such a project. Earlier approaches were based around the placing of random items of food into a neutron beam, exclaiming that they scatter and then approaching industry to hand over some cash. A different approach seemed more appropriate and this led to meetings with Peter Lillford, at that time on a McMaster Fellowship with CSIRO from the UK. Peter had many years of experience working for Unilever, was a former colleague of Stuart's, and was precisely the person from whom to bounce ideas in order to develop a robust program using neutron scattering. Incidentally, Peter had performed experiments at Harwell in 1974 with John White measuring the inelastic scattering of poly(lysine).

A number of meetings were arranged with potential collaborators at CSIRO Food-Futures Flagship, Preventative-Health Flagship, Human Nutrition (it has undergone several name changes in the interim) and Food Science Australia (at that time, a joint venture between CSIRO and the Victorian Government). Further meetings took place with Mike Gidley at the University of Queensland and who is also another member of what we jokingly describe as the Unilever mafia (i.e. the large number of ex-UK or ex-Netherlands researchers who have made their way to Australia, or indeed, New Zealand). Letters were obtained from these organisations and to support the proposal for the 'application of scattering based methods to investigate fundamental and industrial problems in food science'. These initial meetings also led to a proposed short list of four potential projects of which two would be selected, and this was contingent on ANSTO fully funding two postdocs – one dedicated to each selected topic.

Elliot Gilbert and QUOKKA

A project proposal was prepared in March 2005 and then presented formally to ANSTO's Technical Advisory Committee as part of the Bragg Institute's portfolio. This was subsequently approved and led to the preparation of a 'Research Project Summary'. Interestingly, on searching through my files, I find that, in the interim period while 'suitably skilled postdocs' were to be recruited, Tracey Hanley and Andrew Nelson were both going to contribute 50 per cent of their time to the project and Jamie Schulz with 30 per cent of his time. It's good to see that these original, albeit unofficial members, of the project are still at ANSTO and have thrived within the organisation. Advertisements went out in July 2005 and the first offer letters for postdocs went out in October 2005 and January 2006, respectively, although the first experiments started in September. Road-mapping exercises followed with external collaborators.

Those initial projects focussed on understanding the structure of starch and the optimisation of resistant starch (an area in which we continue to work today) and the influence of moisture of the material and functional properties of food-relevant proteins. Even before the project started, we had our first report in the media (2 December 2005, *The Australian*) on what we proposed to study in the starch arena. By April of 2006, I had my first postdoc on board (Catherine Kealley – ex-PhD student of Margaret Elcombe) and, in May, joined by a second (Amparo Lopez-Rubio from Valencia) in just enough time to launch externally the 'Food Science project' on 4 July 2006. This was the signing of the ANSTO-CSIRO-UQ collaboration agreement and resulted in the first of many reports in the media (15 just related to the launch including in *Australian Financial Review*, *Hindu Times* and the *Beijing People's Daily*) as well as the national news broadcast. It's not every day that someone is going to save the world by exposing food to neutrons! The first conference presentation was in May 2006 and first paper emerged in December 2006. In addition, we organised a successful micro-symposium on Food Materials Science as an adjunct to The Australian Institute of Food Science and Technology conference with the aim of getting greater exposure to the community.

Those initial projects focussed on understanding the structure of starch and the optimisation of resistant starch

Neutrons and Food conference in Sydney in 2010

The program went from strength-to-strength and a third postdoc, Anna Sokolova (now the instrument scientist for the next SANS instrument, BILBY) was recruited in June 2007. More publications, media reports and conferences followed and we also seemed to be making some in-roads into convincing the broader community to jump on-board. By the end of 2007, we had eight publications and seven more on the way, new international collaborators and even a mention by the then Science Minister, Julie Bishop, in Parliament.

With our collaborators at CSIRO, Food Science Australia and Queensland, we then looked into formally approaching industry and this lead to the setting up of the 'Protein Syndicate', which seven companies joined and paid a membership fee to access our research on a range of food-relevant proteins at low moisture. These companies were domestic and international and covered the broad spectrum of protein classes. The income from this enabled the employment of joint postdocs. The original name was 'Protein Club' but this was considered to be unlikely to be approved by the senior managers within these companies as the name had connotations of a country club instead of a scientifically-robust outfit.

We wrote the first review on the application of neutron scattering to food in 2009, and this was published in the prestigious journal '*Trends in Food Science and Technology*'. One of the objectives for the program was to address what was considered to be an as-yet untapped market for food scientists using neutrons. In the first open round for time on QUOKKA (my other and, I was repeatedly reminded, the more important of my jobs) it was comforting to see that 10 per cent of all beamtime requested was food materials science related which subsequently increased to 20 per cent and, indeed, the first publication from QUOKKA, was related to the study of starch.

In late 2010, we organised 'Neutrons and Food: Addressing the challenges of food science in an evolving global environment using novel methods' in Sydney. This meeting was supported by the Department of Innovation, Industry, Science and Research, under its International Science Linkages Program, in partnership with the European Union's NMI-3 Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy as well as Oak Ridge National Laboratory, and formed the basis for the 2012 'Neutrons and Food 2' meeting at Delft. We have also continued in the theme of working with industry, now having generated publications with Unilever (on the structure of cholesterol-lowering structuring agents in emulsions) and Perten, a local company. The latter was to modify an industrial testing unit so viscosity data could be obtained simultaneously with SANS.

Judging by the commendations, invitations and perception, it's clear that we have truly placed ANSTO at the forefront of food materials science on a global scale. On reflection, with the critical resources of six postdocs that have come and gone through the group as well as year-in-industry, summer students, visiting fellows and PhD students, we've had a pretty successful time and are now looking forward to postdoctoral fellow number seven. Watch this space.

Energy materials research at the Bragg Institute

Vanessa Peterson

The Energy Materials project is a formal research project at the Bragg Institute focussed on progressing new sustainable-energy technologies through the coupling of neutron-scattering tools and experts at the Bragg Institute with external collaborators.

Creating a global energy-system that is both environmentally and economically sustainable is one of the greatest challenges currently facing scientific and engineering communities. Alternative energy sources, new materials, and gas separation and sequestration technologies have risen as a result of the combined needs for energy and environmental sustainability, with the focus moving increasingly away from fossil fuels. Neutron scattering represents a wide range of analysis techniques that have made important contributions to each of these areas. Energy materials research addresses issues of global importance, whose concepts are accessible by the broader non-research community. The project therefore stands as an excellent example of the usefulness and purpose of neutron scattering to the general public, of great importance to ANSTO.

At the practical level, the project functions as a club where members share knowledge of the materials themselves and the idiosyncrasies of their analyses using neutrons – tools and tricks in experimental approaches. Energy materials research was well established prior to the commencement of the project formally, with the project looking to leverage existing research to reach further for higher impact research results through a coherent and consolidated approach – where the project's productivity is greater than the sum of its parts.

The Energy Materials project was initially known as The Neutrons for The Hydrogen Economy project, with research focussed around using hydrogen as an alternative energy carrier, and its research scope encompassing hydrogen production, storage, and use in fuel cells. The need for battery materials as part of an integrated energy storage system was widely recognised and included in this early vision.

It was clear from the outset that a large community already existed in these research areas, and along with this was a substantial gap between this community and the infrastructure available at the Bragg Institute, with many researchers entirely new to large-scale-facility use. A National Community Focus Day was held at the OPAL Auditorium, on 22 June 2007, with the purpose of receiving input to help direct the project's research, highlight community research so that the project could effectively invest in resources to serve internal research interests and those of the community, and to create opportunities to form collaborative links with external expertise and groups.

Attendees of the National Community Focus Day 2007

Sessions were held in three research areas: Hydrogen production, hydrogen storage, and energy production (encompassing fuel cells and batteries). Both high-level economic and low-level research drivers and barriers were presented in focus areas.

The National Community Focus Day coincided with the commissioning of the OPAL reactor and the first neutron scattering instruments, formally recognising the link between this landmark infrastructure and the energy materials research community to which it is so useful. In doing so, the workshop formally launched the project.

The project, by its nature, is highly collaborative. Many attendees of the National Community Focus Day were entirely new to large scale facility use, and as a direct result of the event, major research projects were launched with three new collaborator groups. These collaborations have been exceptionally fruitful, expanding to ongoing research agreements

	Hydrogen production	Battery materials	Gas storage/ separation materials	Fuel cell materials	Solar cell materials
2010		1 (5.0)	3 (8.1)	1 (2.2)	2 (2.3)
2011	1 (4.1)	10 (4.4)	5 (5.7)	1 (10.2)	1 (3.7)
2012 (to Nov)	1 (5.2)	8 (4.0)	4 (10.8)		1 (TBA)

through the involvement of joint ANSTO-collaborator graduate researchers and postdocs. The project and its collaborators have produced excellent research results, with these published in respected peer-reviewed journals as outlined in the table (above), where the average impact factor is shown in parentheses.

Many of these results were enabled through state-of-the-art instrumentation available at the Bragg Institute. *In-situ* experimentation has a large role to play in this research, with instruments such as WOMBAT (the high-intensity powder diffractometer) playing a crucial role in understanding the atomic and molecular-scale functionality of these materials by providing structural information for materials in real time as they function.

A good example of this is the project's battery research program, which has been strongly driven by insights into electrode functionality revealed by WOMBAT. Some highlights of this research include the discovery of the complementarity between two anode materials – where the two electrode materials were found to function at different voltages, leading to a broader voltage range for the battery through use of the composite material. This result was published with a graduate researcher from a group new to neutrons entirely as first author (G. Du *et al.*, *Advanced Functional Materials* 21, 3990–3997 (2011)). More recently investigations by the same group into the next-generation cathode material $LiFePO_4$ revealed the details of its delithiation pathway. Using WOMBAT the simultaneous occurrence of solid-solution and two-phase reactions was identified after deep discharge in non-equilibrium conditions. This work is an example of the importance in studying non-equilibrium states in such materials and was published with a project post-doc as first author (N. Sharma *et al.*, *Journal of the American Chemical Society*, 134, 7867−7873 (2012)).

Similarly, the project has produced some outstanding discoveries concerning materials being used for the separation and storage of gases that are of use in the energy sector, including for hydrogen, carbon dioxide, and oxygen. Much of the experimental work required to achieve such results are complicated by the *in-situ* nature of the experiments, which often require complex environments. Specialist equipment developed as part of the project is key to progressing this research using neutron scattering. Such equipment, developed with this research community in mind, resulted in the first Science paper produced from the neutron scattering instruments (E. Bloch et al., Science 335, 1606-1610 (2012)), where external and Bragg Institute researchers collaborated to study a material with excellent gas-separation capabilities.

The importance of the project's role in progressing gas separation and storage technologies was recognised through an award from the Science and Industry Endowment Fund (SIEF). The team of researchers was awarded $6 million to develop advanced metal-organic framework materials to capture and convert carbon dioxide. The team combines excellence in materials synthesis, characterisation, and engineering, and includes leading researchers from the Bragg Institute, CSIRO, the University of Sydney, the University of New South Wales, Monash University, the University of Melbourne, the University of Adelaide, and the Cooperative Research Centre for Greenhouse Gas Technologies (CO2CRC). The funds support equipment and postdoctoral researchers for the project.

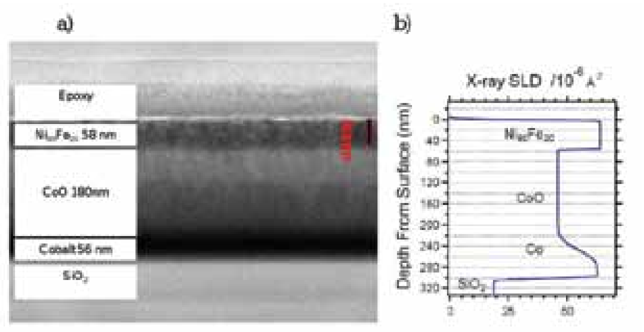
The SIEF-funded 'Solving the Energy Waste Roadblock' research team

Computational calculations yield important insight into the functionality of materials, and are particularly relevant to energy-materials research. The neutron scattering experimental efforts of the project are complemented by a range of atomistic computational calculations, with such calculations being of particular importance in understanding neutron spectroscopy measurements. The project has invested in resources (hardware, software and people) to meet the community's needs in this area. Many of the project's research achievements and discoveries were enabled through these resources.

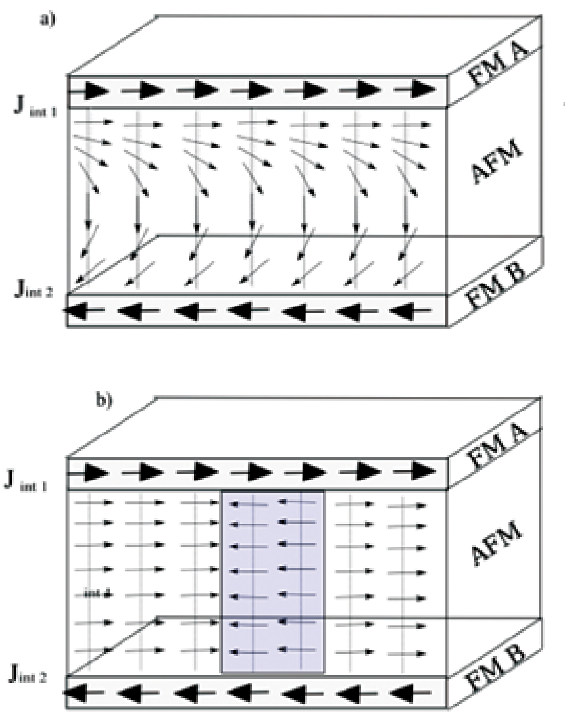
Overall, the project is flourishing and has a healthy outlook for the future as new neutron instrumentation becomes available at the Bragg Institute, particularly with respect to spectroscopic information – which is currently gained at overseas facilities.

Thin film magnetism at the Bragg Institute

David Cortie and Frank Klose



Comparing electron microscope image with X-ray reflectivity depth profile in permalloy/CoO/Co tri layers

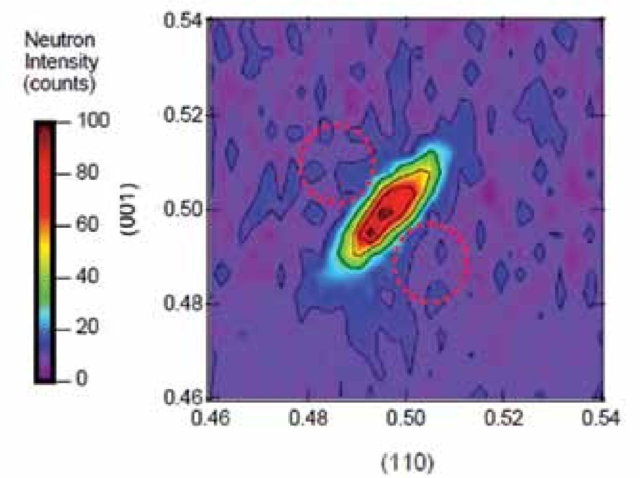


Models for magnetic coupling of ferromagnetic layer through an antiferromagnetic space layer

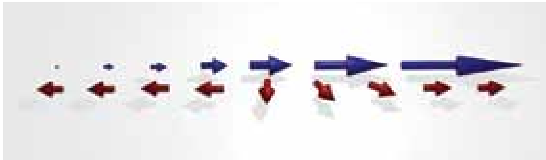
It has been an exciting decade for researchers working in magnetic thin film science: the first Nobel Prize in this area was awarded in 2007 to Fert and Grünberg in recognition of their discovery of interlayer coupling and giant magneto-resistance in Fe/Cr multilayers. Their work set in motion a chain of inventions that has changed irreversibly the lives of ordinary people, by increasing dramatically the amount of data that could be stored in personal computers; one terabyte magnetic hard-disks that are now routinely available! Amidst this climate of innovation, research accelerated into a wide range of systems showing a useful interplay of magnetism and electron current, leading to a new technological paradigm: spintronics. Energy efficiency, increased computing power and access to quantum algorithms are the ultimate goals of spintronics, a field which, although still in the process of birth, may eventually replace traditional semiconducting technology.

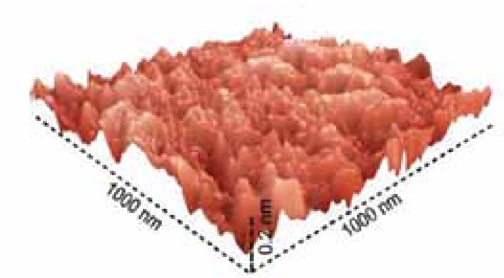
Our group at the Bragg Institute has aimed at refining the art of using neutron techniques to study magnetic thin film nanostructures, with a particular interest in materials that show potential for spintronics applications. Candidate materials for these high-tech pursuits remain scarce, and it is essential to investigate the magnetic behaviour 'beneath the surface' – a task to which neutrons are particularly well suited. During the past few years, we have made extensive use of the instrumentation at ANSTO including the brand-new neutron spectrometer (TAIPAN) and polarized neutron reflectometer (PLATYPUS) which have made it possible to study magnetic thin-film systems using neutron techniques for the first time at OPAL. The main areas of study have been the interlayer coupling, similar to that discovered by Fert, magnetic exchange bias (as used in contemporary magnetic hard-drives), multiferroic materials (as envisioned for multistate memory) and ferromagnetic semiconductors (to bridge conventional and spintronics circuitry). These topics are linked thematically to the goals of spintronics, but are also fascinating playgrounds to explore the fundamental magnetic exchange interactions, and magnetic frustration, on atomistic scales. Research highlights include the discovery of the origin of unusual biquadratic coupling in Co/CuMn multilayers, induced magnetism in $NI_{80}Fe_{20}/Fe_2O_3$ interfaces, and some of the first neutron diffraction experiments on antiferromagnetic materials CrAl, $BiFeO_3$ and $BiFe_{0.5}Mn_{0.5}O_3$.

During this time four PhD students have graced the Reactor Beam Hall: Nick Loh, Thomas Saerbeck,



Commensurate magnetic Bragg peak in $BiMn_{0.5}Fe_{0.3}O_3$ on $SrTiO_3$ measured on TAIPAN





An atomic-force microscope image of nanocrystalline haematite/permalloy thin film

David Cortie and Joel Bertinshaw supervised by Frank Klose, Clemens Ulrich and Anton Stampfl. The joint team has played a key role in designing and commissioning the polarisation equipment on the PLATYPUS reflectometer 2010-2011 that culminated in the first publications of polarised data in 2012. These students managed to win a few prizes (Thomas Saerbeck, Best Poster IEEE Magnetic School, Joel Bertinshaw, Best poster Hercules 2011, David Cortie, Best presentation ANU NCTA 2011, AIMM Three Minute Thesis 2012), and enjoyed the three C's of neutron scattering: cadmium, cryostats and caffeine! With the combined power of the OPAL research reactor, state-of-the-art polarisation equipment and the emerging strengths of local universities, we hope to continue to delve into some of the unchartered waters in the field of magnetism and spintronics in the coming decade!

It has been an exciting decade for researchers working in magnetic thin film science

Structure and properties of Technetium compounds with magnetic ordering

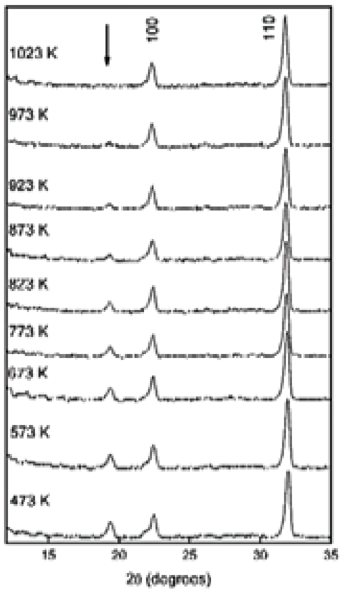
Gordon Thorogood, Brendan Kennedy and Max Avdeev

Technetium is the lightest element that does not have a stable isotope and, hence is not found naturally. Nevertheless it occupies a central position in contemporary nuclear medicine, being one of the most commonly used radiopharmaceuticals. Technetium is also a critical part of the nuclear fuel cycle, and its presence in used fuel elements presents significant challenges in the storage and immobilisation of nuclear waste.

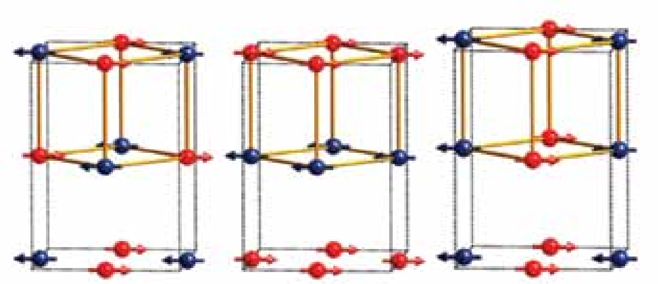
Despite the obvious technological and economic importance of technetium, the fundamental solid state chemistry of this element has been neglected. Technetium has a $5s^2 4d^5$ electron configuration and a range of oxidation states are available, many of which contain 4d electrons. The analogous 4d perovskites $SrMoO_3$ and $SrRuO_3$ have been extensively studied and each shows unique electronic and magnetic properties. The conductivity of $SrMoO_3$ is amongst the highest of all metal oxides, and $SrRuO_3$ is a rare example of a ferromagnetic 4d metal oxide. It might be expected, therefore, that $SrTcO_3$ shows unusual electronic and magnetic properties, but prior to this work just how unusual these were was unclear.

We prepared polycrystalline samples of the two perovskites $SrTcO_3$ and $CaTcO_3$ using the facilities at ANSTO's Institute of Materials Engineering. Subsequently we performed neutron diffraction on the two oxides using the ECHIDNA diffractometer at the OPAL facility. Neutron diffraction has two advantages for this work, firstly it provides great sensitivity to the positions of the oxygen atoms, something that is essential to determine accurate and precise structures of these types of oxides; and secondly neutrons have spin making these ideal to probe the magnetic structures.

Neutron diffraction measurements (figure above right) of both samples demonstrated that they were magnetic at room temperature. Analysis of the high-resolution neutron diffraction data revealed that $SrTcO_3$ adopts a distorted perovskite structure with G-type antiferromagnetic ordering (figure below right) and has a moment of 1.87 µB per Tc cation at room temperature.



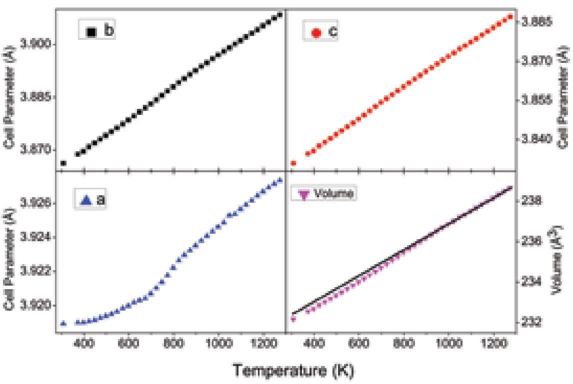
Portions of the observed neutron patterns from $SrTcO_3$ (λ = 1.538Å) illustrating the evolution of magnetic reflections. The 100 and 110 nuclear reflections are indexed on the cubic structure. The arrow shows the progressive decrease in intensity of the orthorhombic (110)+(101) reflections.



(left) G-type antiferromagnetic ordering in the orthorhombic unit cell used for the structural refinement with the NPD data. (centre) The A-type antiferromagnetic ordering and (right) C-type ordering.

Variable temperature neutron diffraction measurements were then performed to establish the Néel temperature of the two oxides. These measurements demonstrated that $SrTcO_3$ is isostructural with $SrRuO_3$ and displays the same sequence of structures upon heating. More remarkable was the Néel temperature, being above 1000K. This is the highest Neel temperature for any metal oxide that does not contain a 3*d* transition metal. $SrRuO_3$ is a ferromagnet with a Curie temperature of 160 K. The high-temperature phase changes were then confirmed via X-ray diffraction at the Australian Synchrotron.

Electronic structure calculations confirmed that the ground state corresponded to G-type antiferromagnetic and that the Fermi energy lies in a clearly defined manifold of Tc t_2g d states, which are considerably hybridized with the oxygen p-π orbitals. These calculations suggest that replacing the Sr with the Ca should result in a reduction in the Néel temperature. This was experimentally verified, using a combination of neutron and synchrotron X-ray diffraction data. A significant difference between $CaTcO_3$ and $SrTcO_3$ was that the former did not display any crystallographic phase transitions upon heating, although evidence for magnetostriction was found, corresponding to a Néel temperature of 600 K.



Temperature dependence of lattice parameters (a, b, and c and the unit volume) for $CaTcO_3$, estimated from Rietveld analysis of synchrotron X-ray diffraction data. The structures were refined in an orthorhombic space group Pnma. The solid line is a linear extrapolation of the high-temperature volume.

The study of the technetium materials is a good illustration of how the co-location of the Institute of Materials Engineering, the Bragg Institute, and the OPAL reactor at Lucas Heights creates a combination of facilities and expertise of unparalleled potential, to make world-class discoveries in the structure and physical properties of materials with exotic and radioactive elements.

A combination of facilities and expertise of unparalleled potential, to make world-class discoveries

Reflecting on neutron studies of organic optoelectronics devices

Paul Burn, Ian Gentle and Michael James

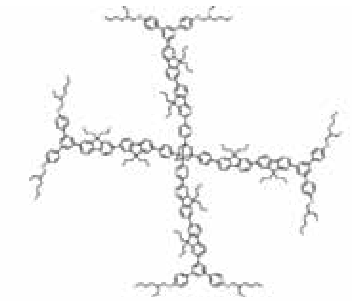
Optoelectronic devices come in many shapes, sizes and functions; and are now a ubiquitous part of our everyday lives. Conductive organic compounds have been researched since the 1950s and 60s, with significant advances being made in the late 1970s by Heeger, MacDiarmid, and Shirakawa leading to the award of their 2000 Nobel Prize in Chemistry. Alongside these advances, Ching W. Tang while working at Eastman Kodak, pioneered the development of conducting organic materials that interact with light; notably the organic light-emitting diode (OLED) and the heterojunction organic photovoltaic (OPV) solar cell.

Organic conductors and conducting polymers are lighter, more flexible and generally less expensive than traditional inorganic conductors, creating the possibility of new applications that would not be possible using conductors such as copper or silicon. Aside from OLEDs (used widely in smart devices and flat panel displays) and OPVs, new applications for optoelectronics are also being envisaged such as electronic paper, smart windows and also show potential for use in molecular computers. Common to almost all of these devices is that organic molecules are arranged into thin films on the nanoscale, making them particularly well suited for study using neutron reflectometry.

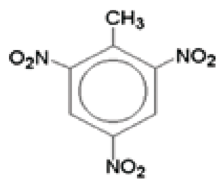
One of the most productive research areas associated with neutron reflectometry at OPAL has been the study of the structures, morphologies and properties of a range of optoelectronic thin-film devices, in collaboration with the University of Queensland's Centre for Organic Photonics and Electronics (COPE), the National Deuteration Facility and the Bragg Institute. While the capabilities that have been developed for *in-situ* time-resolved neutron reflectometry using the PLATYPUS reflectometer are generic and applicable to many nanoscale thin-film systems, they have been extensively used in three key areas of optoelectronic research: studies of dendrimer-based thin film explosive sensors; studies of molecular interdiffusion in OLEDs; and investigations of the molecular morphology in solution-processed OPVs.

When explosives are welcome at your nuclear reactor…

Events on Northwest Airlines Flight 235 from Amsterdam to Detroit on Christmas Day 2009, saw airport security again become headline news. The introduction of full body scanning at major international airports followed closely in its wake. The need for less invasive, more portable, yet highly sensitive screening methods for explosive materials is of supreme importance to security agencies. The team at COPE has developed a range of new fluorescent dendrimer molecules that can be solution-processed into thin films and used as solid-state sensors to detect vapours from explosive molecules using oxidative luminescence quenching. In the absence of an explosive analyte and in the presence of ultra-violet light, these sensor films fluoresce to produce light in the visible spectrum. When exposed to vapours from explosives such as trinitrotoluene (TNT, Figure 1b) and its analogues, para-nitrotoluene (pNT) or 2,4-dinitrotoluene (dNT), the photoluminescence from the dendrimers is quenched by as much as 90% in just a few seconds.



A 3-dimensional photoluminescent dendrimer comprised of four bifluorene units arranged around an adamantyl centre;



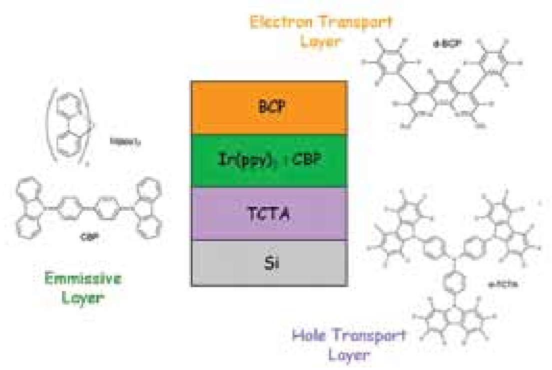
Trinitrotoluene.

Combined *in-situ* fluorescence spectroscopy and neutron reflectometry measurements were made using PLATYPUS for both pristine and analyte-saturated films, which gave important insights into the analyte adsorption processes and molecular interactions within these sensors. As shown above, both dendrimer and analyte are based on similar aromatic molecular motifs which means that the way in which they scatter neutrons is very similar. In order to make the analyte molecules more visible to neutrons amongst the dendrimers it was necessary to use deuterated forms of pNT and dNT to improve the scattering contrast. Neutron reflectometry revealed nanoscale swelling of the thin dendrimer films during analyte adsorption, and was also able to quantify the quantity and distribution of analyte within the sensor films. From the reflectometry data, it was also clear that a single analyte molecule was able to quench the photoluminescence from more than one dendrimer molecule. On removal of the analyte from the films, by blowing with nitrogen, a range of behaviours were observed depending upon the combination of analyte and dendrimer. In most instances, the films returned to their original thickness and scattering length density; yet to differing extents, trace amounts of analyte led to different levels of restoration of photoluminescence from very little to essentially fully reversible.

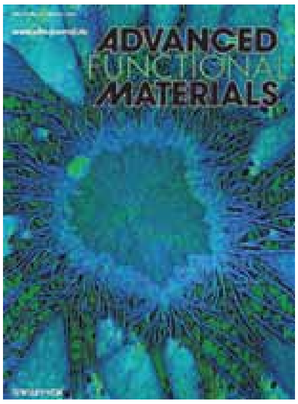
Optoelectronic devices are now a ubiquitous part of our everyday lives

Shedding light on nanoscale diffusion in OLEDs

While the operating efficiencies of thin-film organic light-emitting diodes are extremely high (approaching 100 per cent), their lifetimes require significant improvement before the widespread use of such devices. OLEDs rely on the separation of charge in discrete layers within a nanoscale thin film (above right) and the stability of these molecular layers under operational conditions is essential for optimum performance. To better understand the morphologies and molecular interactions within a range of OLEDs, as-prepared and annealed devices were investigated in a series of experiments using PLATYPUS. A purpose-built cell allowed *in-situ* annealing and simultaneous collection of photoluminescence and



A trilayer OLED device, consisting of ~30 nm thick discrete molecular layers. The electron- and hole-transport layers have been selectively deuterated to provide scattering contrast with the light-emitting layer.



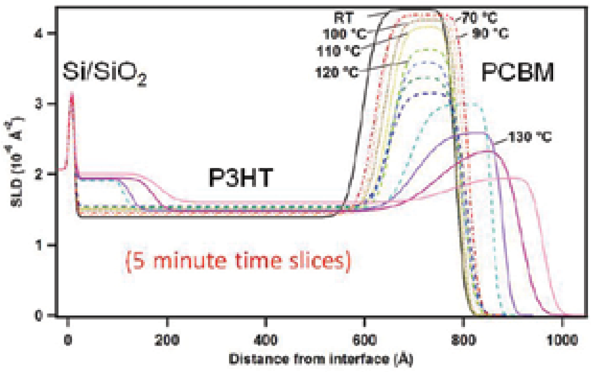
Composite photoluminescence microscopy image of phase separation of Ir(ppy)3 complex and CBP in the emissive layer upon thermal annealing.

neutron reflectivity data. Scattering contrast between key molecular components in the hole-transport layer, the electron transport layer and the light emitting layer was enhanced using chemical deuteration.

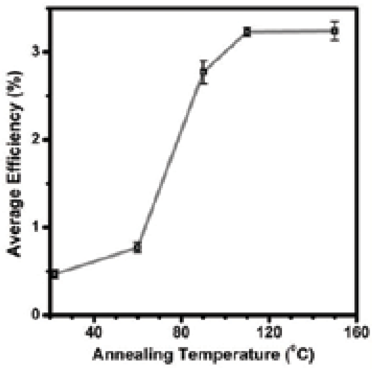
Phase separation was found to occur upon annealing in the light-emitting layer between the iridium complex and the molecular host, as revealed in the cover image of the June 2011 issue of journal *Advanced Functional Materials*. Inter-diffusion between the electron transport and emissive layers within the multilayer stack was found to occur upon annealing; while the interface between the emissive- and hole-transport layers was found to remain intact. In a series of studies we were able to characterise the diffusion processes, quantify the degree of intermixing and correlate the results with the amount of solid state emission from these devices.

Untangling the nanostructures of OPVs

While discrete molecular layers are essential for high-performance OLEDs, the converse is true for organic photovoltaic solar cells (OPVs). The best performance



Neutron scattering length density profile of a solution processed bilayer sample of PCBM on P3HT on silicon as a function annealing. Significant interdiffusion between the two layers occurs above 120 °C.



Increasing efficiency of these OPV solar cells with annealing, indicating little improvement above 110 °C.

in OPVs comes from molecular structures called bulk heterojunctions, where electron-donor (e.g. conducting polymers like poly-3-hexyl thiophene (P3HT)) and electron-acceptor materials (e.g. fullerene-based such as PCBM-C60) are blended on the nanoscale within the active layer of the device. In these types of solar cells, light generates excitons that lead to a separation of charges at the interface between the donor and acceptor materials. These charges then flow to the electrodes of the device where they are collected to perform work.

The team at COPE has developed methods for producing OPVs by solution casting individual layers of donor and acceptor molecules. OPVs produced by solution processing methods typically show poor efficiencies in their as-cast state, and require annealing at temperature in order to form bulk heterojunction structures and improve their efficiencies. Time-resolved neutron reflection in conjunction with *in situ* annealing allowed the investigation of the molecular inter-diffusion of donor and acceptor molecules throughout the thin films of OPV devices. Importantly, neutron reflectivity measurements on as-cast samples reveal significant inter-diffusion of the PCBM acceptor molecules into the lower P3HT donor molecule layer even before annealing. Devices annealed at temperatures up to 150°C showed essentially complete inter-diffusion accompanied by substantial increases in their external quantum efficiencies. Importantly, large gains in efficiency seemed not to require complete blending of the bilayer structure, but only modest increases in the amount of PCBM acceptor in the largely P3HT donor layers. Photovoltaic devices fabricated using this bilayer approach and suitable annealing conditions (including those formed by photocrosslinked P3HT) yielded comparable power conversion efficiencies to pre-blended bulk heterojunction devices made from the same materials.

Modern diffraction methods for the investigation of thermo-mechanical processing

Klaus-Dieter Liss

ECHIDNA , Lareine Yeoh and Klaus-Dieter Liss

Engineering-related materials science was an important consideration as the first suite of instruments at OPAL was defined. Among these, the neutron strain scanner, KOWARI, was set up with state-of-the-art definition of a gauge volume under 90° diffraction angle and with a 2-dimensional detector. The hardware comprises a heavy-load x-y-z sample table, and a mechanical load frame was included in the project. Oliver Kirstein was hired in 2002, from Germany to lead the KOWARI construction project. Vladimir Luzin, an expert in texture and strain scanning, also joined ANSTO in 2006 for the operational phase of the KOWARI diffractometer. When Oliver Kirstein left ANSTO in 2011, Anna Paradowska joined the Institute from the ISIS spallation neutron source in the United Kingdom.

In addition to the interests of the engineering and strain-scanning community, the profile of 'thermo-mechanical processing' was raised when I arrived, with a strong background in the use of synchrotron high-energy X-rays, another metal-penetrating radiation. I had been in charge of the ID15A beamline at the European Synchrotron Radiation Facility, in France, and had done early materials-science experiments there with both Alain Jacques, from Nancy, and Reimer's group from Berlin. On joining ANSTO to complete the construction of the ECHIDNA High-Resolution Powder Diffractometer, I initiated the idea of texture measurements using ANSTO's powder diffractometers. Initial measurements were attempted at HIFAR's 2tanA and TASS instruments, together with Andrew Studer. An old X-ray Eulerian cradle was adapted and connected to the instrument, for initial measurements on well-studied Ti-Al samples, allowing the diagnosis of problems and to establish the orientation mapping algorithm. Another approach was taken using the AUSANS small-angle scattering instrument for the investigation of precipitation processes in metallic systems, based on the experience of Robert Knott.

During the construction of ECHIDNA, I continued high-temperature *in-situ* studies on titanium-aluminium intermetallic compounds, using high-energy synchrotron X-rays at the ESRF in France. This type of transformation study was on the list of the first 10 experiments to be done on the ECHIDNA machine. Complementary ideas for combustion synthesis occurred for the usage of WOMBAT, driven by Erich Kisi (Newcastle University), member of the Instrument Advisory Team, and his former student Daniel Riley. Ian Madsen (CSIRO), another member of the Instrument Advisory Team, represented the ideas of industry-related high-temperature studies for the reduction and production of metals.

After careful study of the opportunities with the potential Australian clientele, I proposed a project on the studies regarding thermo-mechanical processing. My background in materials science was light, just like my university counterparts' background in diffraction analysis. In giving presentations all over the country, I met people who had interesting problems and were fascinated by the methods, just as much as I was excited by the rolling process of a hot glowing piece of metal. I realised that there must be potential behind this, if we could achieve mutual understanding, learn from each other and trust. Besides an existing overseas collaboration with Helmut Clemens (Leoben, Austria), ANSTO was by 2004 working with Rian Dippenaar at the University of Wollongong and his team, who were working on metals at high temperature using Laser Scanning Confocal Microscopy. A small project at ANSTO expanded with a year-in-industry student, LaReine

KOWARI (with 640kg sample from the Welding Institute, UK)

Yeoh, who was succeeded by Ross Whitfield, Ian Watson and Lewis Ryan over the following four years. Interest was raised and critical mass acquired to propose a project entitled *Modern Diffraction Methods for the Investigation of Thermo-Mechanical Processes*. This resulted in an ANSTO Senior Research Fellowship, attached to the Bragg Institute, starting in 2007.

PhD Student Kun Yan and postdoc Ulf Garbe were then hired by the project, to develop and implement the early stages of research and measurements at OPAL. We undertook our first hot-plastic-deformation studies in 2008 at the Advanced Photon Source (APS) synchrotron in the USA, where we had been granted beam time through the Australian Synchrotron Research Program. I had never undertaken plastic deformation studies before, just heating, but this was the next logical step. The proposal was on the texture evolution of Zircaloy-4, a nuclear-reactor structural material in which Huijun Li,

A variety of users have been attracted or educated through the project

from ANSTO's Institute of Materials and Engineering Sciences was interested. A second proposal on the same trip was with Elena Pereloma of the University of Wollongong, who contributed with the support of Tom Schambron, who had experience in running physical simulations of thermo-mechanical processing on their Gleeble machine. We took three specimens, carefully prepared and wire-cut, to the APS. The first was ripped apart in a fraction of a second, by false load specifications. With the second sample, we somehow managed to get some idea of the texture components at high temperature, while slow plastic flow was applied. We shortly realised that there were fluctuations in the Debye-Scherrer rings, which seemed somehow regular and fascinating. With one single specimen left, we decided to go for the direct observation of dynamic recrystallisation: we actually performed seven runs on the same sample, each time increasing the mechanical load and approaching step by step the optimal parameters, before we concluded, what was the best and went ahead, until failure of the sample. From these three days of beam time, we produced 300 frames taken in 60 seconds of time only! In these results lie the foundation of *in-situ*, time-resolved diffraction, exploiting not only the classical aspects of powder diffraction, namely quantitative phase, lattice parameter and texture analysis, but also giving insight into grain correlations, grain rotation, grain growth, subgrain formation, dynamic recovery and dynamic recrystallisation. The resulting paper made it onto the cover of *Advanced Engineering Materials*. Two years later, we used the same method to study hot-deformation in a 2-phase Ti-Al based alloy at 1300°C, revealing the co-existing, but very different deformation processes of the two.

Neutron commissioning of the OPAL instruments continued to progress well, and the first *in-situ* heating-cooling cycles were applied to various metals. Ulf Garbe and Oliver Kirstein measured the first pole figure from a copper specimen, which had already been characterized using high-energy X-rays at the ESRF. Together with the synchrotron *in-situ* deformation studies, the first OPAL neutron results were presented on a second journal cover, again in *Advanced Engineering Materials*. The team also set up to do routine texture measurements at the OPAL powder diffractometers, particularly after implementing algorithms for making use out of the large solid angle and reciprocal space coverage of the WOMBAT detector. As Ulf Garbe moved on to become project leader and scientist for the new DINGO imaging beamline, Saurabh Kabra was recruited from Los Alamos into the team. His background in strain, texture and Rietveld analysis was very useful in the implementation of combined Rietveld and texture refinement.

A variety of users have been attracted or educated through the project. Former student, Ross Whitfield, published WOMBAT's first paper on *in-situ* phase transformations while sintering stainless steels. Peter Hodgson, Hossein Beladi and Rakha Khusboo have studied the evolution of transformation-induced plasticity steels, and sample environment including an induction heating-coil and rapid quencher is being developed with the local sample-environment team, led by Paolo Imperia. A succeeding project with PhD candidate Lisa Thoennessen, on the transformation-induced grain refinement in titanium alloys, is being run again with co-supervision by Rian Dippenaar. There is now a steady stream of incoming neutron proposals from external groups. While user support is maintained, our project team has further developed the exploitation at the edge of the methods for pioneering work. Undergraduate student Ian Watson analysed the disappearance of Bragg scattering signal upon the disordering of Ti-Al phases, due to the opposite signs of scattering lengths of similar magnitude, which is now employed by external groups for sintering and alloying studies from powders. Ongoing studies are on the discovery of primary extinction in crystallites, at very high temperatures, which anneal to almost perfect crystals. The time dependence of such intensity permits conclusions on the defect kinetics, such as the annihilation of dislocations or the nucleation and growth of precipitates. While our research may seem fundamental, or just instrumental, it carries the potential of obtaining thermo-mechanical parameters, which are important for modelling the hot-deformation of metals. Our research applies complementary methods, here at ANSTO, in Australia and overseas, such as electron microscopy, laser-scanning confocal microscopy, state-of-the art physical thermo-mechanical simulation (which is not yet done in the beam), high-energy synchrotron X-ray diffraction and time-of-flight analysis at spallation sources. This allows exchange with the newest developments in the world, to retrieve the best ideas and concepts for future developments at ANSTO and in Australia.

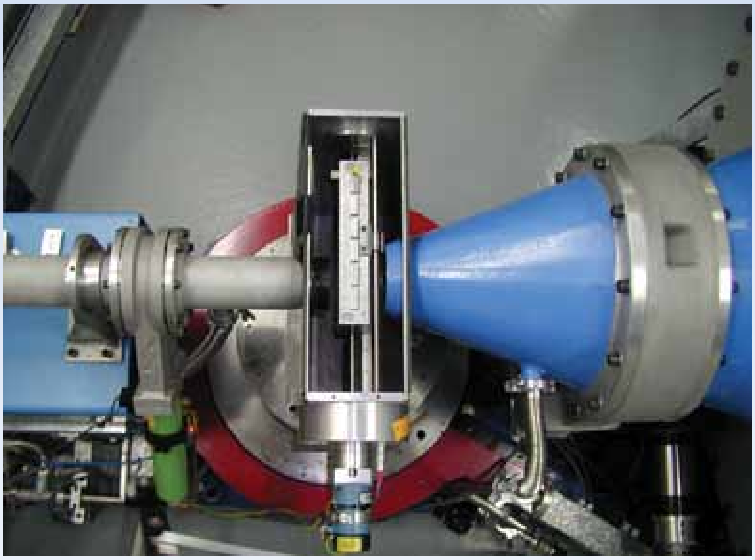
The Bruker SAXS with Jill Trewhella and Rob Robinson

Workshop on “Neutrons for Engineering” at UNSW, September 2002.

Friends in ANSTO-Engineering, with the PLATYPUS collimator box

Second meeting of Bragg Institute Advisory Committee in September 2003 – standing on the site of OPAL's Neutron Guide Hall: left to right: Don Napper, Yasuhiko Fujii, Alan Leadbetter, Rob Robinson, Barry Muddle, George Collins, Mike Rowe, Rob Lamb, Shane Kennedy

Andrew Nelson, instrument scientist for PLATYPUS



Samples on AUSANS at the HIFAR reactor

Our X-ray Reflectometer

The Bragg Institute, ANSTO and Australia's overseas synchrotron programs

Richard Garrett

ANSTO played a pivotal role in the development of Australian use of synchrotron radiation facilities, beginning in 1991 when David Cook (then Executive Director) and John Boldeman assembled a consortium to fund the construction of the Australian National Beamline Facility (ANBF) in Japan. Richard Garrett, David Cookson and Garry Foran were recruited to the project, with David and Garry re-locating to Japan in 1992 as the ANBF beamline scientists.

The Australian Synchrotron Research Program (ASRP) was born when the first Major National Research Facilities (MNRF) program funded additional overseas access for Australia, to the Advanced Photon Source (APS) in Chicago, in addition to continuing the operation of the ANBF. This was a significant step in the development of Australia's user community as the APS was one of the three premier third generation facilities, and the MNRF program provided 5 years of funding certainty. In addition this first MNRF grant included a component earmarked for a feasibility study for an Australian synchrotron. This study, conducted primarily by John Boldeman, grew into the Boomerang proposal and led to the three-state competition to host an Australian light source facility, and to the Victorian announcement in 2001 that it would construct the Australian Synchrotron.

Although the ASRP was somewhat independent from ANSTO (it had its own board), its staff were always employed by ANSTO, initially in the Physics Division. When the Bragg Institute came into being in late 2002, the ASRP staff joined their neutron scattering colleagues in the new Institute. By this time the ASRP had been funded for an additional five years operation under the second MNRF program and had grown to seven staff: Richard Garrett (now Facility Director) and Margaret Edmondson were based at the Bragg Institute, Garry Foran and James Hester were in Japan at the ANBF, and David Cookson, Anton Stampfl and Harry Tong were the beamline staff based at the APS. Soon after the Bragg Institute was established the ASRP added the National Synchrotron Radiation Research Centre (NSRRC) in Taiwan to its overseas facility constituency. Anton Stampfl took on responsibility for the NSRRC user program and Cathy Harland was hired to replace Anton at the APS.

By all measures it was an outstanding success

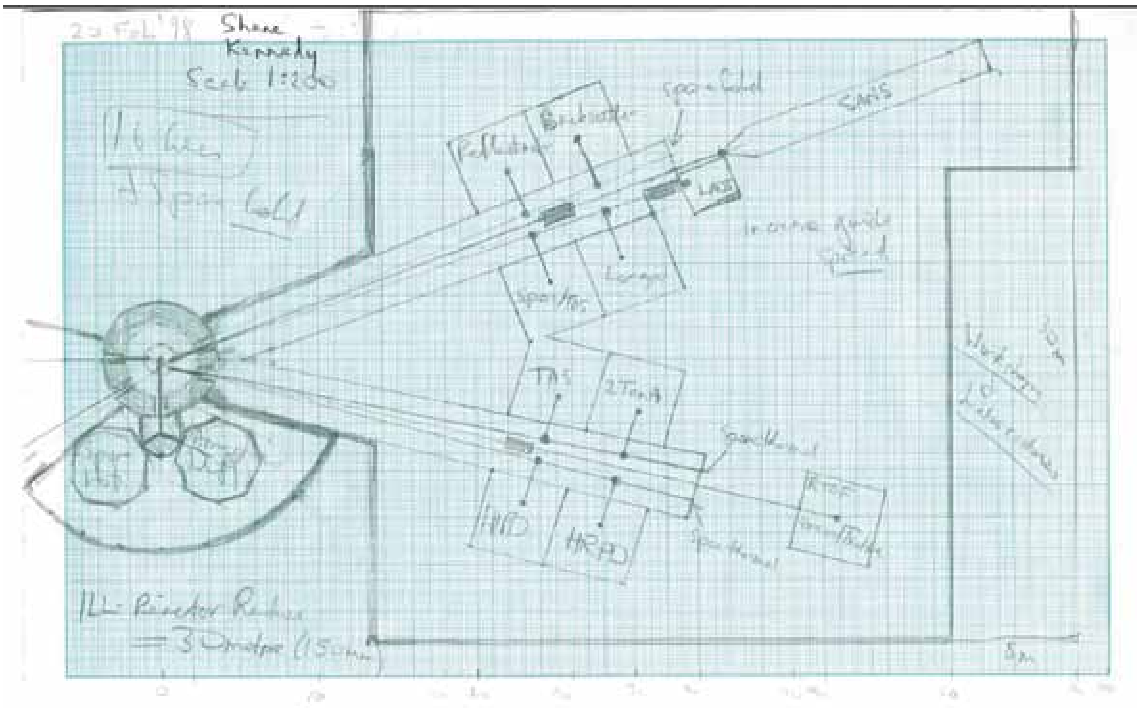
The ASRP program came to an official end in December 2008. By all measures it was an outstanding success: the user program had grown to fill the available capacity at the three overseas facilities with almost 200 Australian user teams performing experiments annually on the ASRP facilities; and over 20 ASRP post-doctoral fellowships were awarded over the 15 years of its existence. The ASRP had both developed the user community and a core of skilled synchrotron scientists in preparation for the establishment of a domestic facility. Of the ASRP staff, Richard Garrett ran the Bragg Institute user program for a short period in 2009 before taking on a broader synchrotron role at ANSTO, Anton Stampfl and James Hester are still with the Bragg Institute having made the transition to neutron beam instrument scientists, David Cookson, Cathy Harland and Bernt Johannessen (who replaced James Hester in Japan in 2007) are at the Australian Synchrotron, Garry Foran is now also working in neutron science at the Japan Proton Accelerator Research Centre facility in Japan, and Harry Tong remains in Chicago.

Opening the soft X-ray end station at the National Synchrotron Radiation Research Centre in Taiwan

While many of the ASRP scientists were only infrequent visitors to ANSTO and their Bragg Institute home base, we all benefited considerably from the establishment of the Institute and the consistent support it provided. More than the similarities in neutron and synchrotron instrumentation, science and their user communities, the ethos and culture of the Bragg Institute neutron scattering and ASRP synchrotron user facilities and their scientific staff was/is almost identical, making the Bragg Institute a natural and happy home for the ASRP for almost 10 years.

The OPAL Neutron Beam Facility and the Neutron Beam Instruments Project (1997-2007)

Shane Kennedy and Rob Robinson



First scale drawing of the OPAL neutron beam facility, based on deliberations of the BFCG (SJK Feb 1998).

When the Australian Federal Government approved construction of a research reactor to replace HIFAR in 1997, the Australian condensed-matter research community finally had the trigger to bring our neutron-beam research capability back to world standard. For the small neutron scattering group at HIFAR, this resulted in an immediate refocus of effort, in order to manage the scoping and design of the beam facility for the new reactor, while still operating a user program at HIFAR. The first step, which was initiated by ANSTO's CEO, Helen Garnett, was to form the Beam Facilities Consultative Group (BFCG) for the purpose of scoping out the key scientific challenges, to define the key requirements for neutron sources, beam transport systems and neutron scattering instruments, and to consider the space requirements for the facility. The members of the BFCG were:

Stephen Burke, DSTO

David Craik, University of Queensland

Andrea Gerson, University of South Australia

Evan Gray, Griffith University

Bob Harrison, ANSTO

Trevor Hicks, Monash University

Shane Kennedy, ANSTO, (Secretary)

Tony Klein, University of Melbourne

Brian O'Connor, Curtin University

Ezio Rizzardo, CSIRO

Gerald Roach, ALCOA of Australia Limited

Claudio Tuniz, ANSTO, (Chair)

John White, Australian National University.

The BFCG completed its work within 6 months, tabling its report in April 1998. Along the way, they drafted the first 'engineering drawing' for the OPAL reactor, shown above. This layout reflected our desire for separation of neutron beam applications from other uses of the reactor (such as radioisotope and NDT Silicon production), and the outcomes of our deliberations on the efficient transport of cold and thermal neutrons away from the reactor face. The layout included space for 17 neutron beam instruments and made provision for later addition of a second neutron guide hall, feeding from the same cold neutron source. The BFCG further developed this concept into the reference design for the tendering process for construction of the reactor, and later for our detailed design of the beam facility, its neutron guide system and its suite of neutron beam instruments.

The principle for construction of the neutron beam facility, as proposed by the BFCG, was to ensure that each instrument was competitive with the world's best existing instrument in its class. This principle guided us in the design of each instrument just as it did in the design of the neutron sources and transport systems for the OPAL reactor itself. For example, one innovation in beam transport system design that gave us a competitive edge in powder diffraction was the installation of a 300 mm high curved neutron guide, with reflective supermirror coatings that delivered intensity gains to the powder diffractometers (WOMBAT and ECHIDNA) through vertical beam focussing by the monochromators. This same principle led us to define the contract deliverables for the reactor construction in terms of performance rather than by technical specifications. This approach proved highly effective in terms of neutron flux delivery to the instruments, by providing the motivation for all parties (designers from ANSTO, INVAP, PNPI and Mirrotron) to collaborate in an integrated optimisation of the design of sources, guide systems and instrument optics.

The original goal was to build eight neutron beam instruments by mid-2005, when the OPAL Reactor was expected to reach criticality, all for $29.4 million (at 1997 rates). This sum was indexed to Department of Finance inflation indicators, and the Commonwealth assumed the risk of adverse exchange rate changes. From a formal point of view, the funding was part of the construction appropriation for the OPAL reactor and while the reactor, cold source, supermirror guides and buildings were included in a large turnkey contract with the Argentinian company INVAP S.E., along with their subcontractors, ANSTO decided to project manage the instrument construction itself.

The initial set of instruments for OPAL were:

1. High-Resolution Powder Diffractometer (ECHIDNA)
2. High-Intensity Powder Diffractometer (WOMBAT)
3. Laue Diffractometer (KOALA)

The original goal was to build eight neutron beam instruments by mid-2005

4. Reflectometer (PLATYPUS)
5. Residual-Stress Diffractometer (KOWARI)
6. Small-Angle Neutron Scattering (QUOKKA)
7. Thermal 3-Axis Spectrometer (TAIPAN)
8. Polarisation-Analysis Spectrometer (PELICAN)

The original plan was to build six new instruments and to do the other two instruments (ECHIDNA and PELICAN) "on the cheap", by moving them from HIFAR. But in the end, seven instruments were constructed from scratch and at an internationally competitive standard, and the eighth eventually became PELICAN, once CEO Ian Smith decided to commit further ANSTO funds in 2005.

The principle of project management for the Neutron Beam Instruments Project was that one scientist would lead each instrument development, with ultimate responsibility for performance, budget and schedule. This approach was driven by the goal to achieve the best performance, by ensuring complete ownership of the project and its outcomes for operational excellence by the instrument scientist.

When the Bragg Institute was formed in December 2002, the Neutron Beam Instruments Project had already been running for two and a half years, and it would continue until a successful conclusion in July 2007 when we conducted a lessons-learnt exercise for all staff involved.

The management team for the project consisted of Shane Kennedy (Project Leader and Scientific Team Leader), Sungjoong Kim (Project Engineer), Kevin Morrison (Business Manager), Greg Whitbourn (OPAL Project Manager) and Rob Robinson (Scientific Manager). Greg had recently joined the Replacement Research Reactor Project (as it was known then), as overall project manager, and he had previously project managed the whole of the electrical installation for the 2000 Olympic Games in Sydney, for Energy Australia.

We were advised every six months by the Beam Instruments Advisory Group, which had grown out of the BFCG, chaired by Tony Klein (University of Melbourne), with the other members at the time being: Yasuhiko Fujii (University of Tokyo), Ian Gentle (President of ANBUG), Evan Gray (Griffith University), Rod Hill (CSIRO), Gerald Roach (Alcoa), Sunil Sinha (University of California San Diego), Lou Vance (ANSTO-Materials) and John White (Australian National University). Dan Neumann (NIST) joined the committee later in 2002, as a replacement for Sunil Sinha, and has advised us on and off ever since.

Aside from Shane and Rob, three of our scientists were with the project from beginning to end: Mike James (who built the PLATYPUS reflectometer), Elliot Gilbert (who built the QUOKKA small-angle neutron scattering instrument) and Oliver Kirstein (who built the KOWARI strain scanner, but has since moved on to bigger and better things at the European Spallation Source in Lund, Sweden). In addition, Nick Hauser and Frank Darmann were with the team from beginning to end. Nick and Frank respectively led the IT/Data Acquisition and Electrical Engineering efforts, once they were split out from the individual instrument projects.

In February 2003, the OPAL Reactor itself was 31 per cent complete and the RRRP project was recovering from a 6-month delay in construction due to the discovery of a geological fault in the excavation for the reactor.

Meanwhile concept design of the cold neutron source, beam tubes was complete, the basic design of the neutron guide systems had been fixed, and we were working on the details of the neutron guide hall, instrument cabins, the layout of services to the instruments, and the laboratories that were to serve the user program. Six out of eight instruments had approved budget/schedule/scope combinations, with the strain scanner (KOWARI) and polarisation-analysis spectrometer (that eventually evolved into PELICAN) yet to be approved in detail. In fact, the February 2003 meeting reviewed the budget, schedule and scope for the KOWARI strain scanner, following a community workshop the previous September and Oliver Kirstein's arrival as instrument scientist. It also reviewed the scope of IT and electrical work, following Nick Hauser's arrival. We had also just settled on the naming convention that OPAL's instruments should not have acronyms as names, but should be named after Australian fauna. This convention seems to have stood the test of time, especially with the public and politicians, although it was not universally popular at the time. Looking back at the reports from this time, we were clearly struggling in the labour market to hire a few of the scientific staff needed, in a timely fashion. Indeed, in one case, we unsuccessfully offered the job to six candidates over three rounds of advertising, before getting anyone suitable to accept. But in time we benefitted from the downturn in the scientific labour market in Germany, and we managed to hire a number of scientists based there, particularly when three of our instrument scientists (Leo Cussen, Brett Hunter and Mark Hagen) left us in quick succession in the course of 2003.

As part of the February 2003 Advisory Group meeting, a clear case for having an ultra-SANS instrument (now called KOOKABURRA) was made by Andrzej Radlinski (then at Geosciences Australia), and this is something that we were eventually able to do with ANSTO funds after the end of the Neutron Beam Instruments Project.

One formidable challenge for the project resulted from the need to obtain a separate nuclear source license for each neutron beam instrument. This was not only a first for ANSTO, but a first for any neutron beam facility worldwide. The process required a complete rethink of the radiation safety standards and procedures that had applied in the HIFAR era, and involved extensive consultation with experts in engineering and safety at ANSTO and with ARPANSA (Australia's nuclear regulator). As a result the Bragg Institute now operates with radiation safety standards as stringent as any user facility in the world.

Other major things that took place during the project were:

- the continual dialogue (and slow improvement) regarding security/access issues at ANSTO and the user community's efforts to try to bring ANSTO and OPAL more into line with practice at other international scientific user facilities
- the case for a dedicated Bragg Institute Office Building (eventually B87), which had been excluded from the original scope for OPAL mid-way through contract negotiations

The Neutron Beam Instruments under construction

- the decision in 2005 by then CEO Ian Smith to "go for gold" with the eighth instrument (eventually the PELICAN time-of-flight spectrometer), once we reached consensus that the original idea of moving LONGPOL from HIFAR to OPAL made little sense
- a substantial and successful effort to get clean earthing built into OPAL's Guide Hall and Reactor Beam Hall
- the decision to go with all-digital control and safety-interlock systems
- strong standardisation of both sample environments and software
- a reasonable investment in sample-environment equipment.

Eventually, the OPAL reactor reached criticality in August 2006 and the first two diffractometers took neutron data in late 2006 and early 2007 respectively. The first paper from ECHIDNA was published in late 2007. Two further instruments took data in mid-2007, but then OPAL experienced major problems with its fuel, and was shut down for 11 months, delaying commissioning of these and the other instruments. But we got back on track again soon afterwards.

In light of the complexity of building a suite of neutron beam instruments concurrently with construction of a multipurpose nuclear research reactor, and the added complications due to delays in the reactor construction, our project completion date of July 2007 stands as a proud achievement for the many ANSTO staff involved.

In order to wrap the project up at its end, we held a Lessons-Learnt Exercise (and celebration) on Friday 17 August 2007 at the Rydges Hotel, Cronulla, with the by-line: "Think Big, Show no Fear, and Stay the Course! Teamwork by Scientists and Engineers." For many of us, this project was the highlight of our careers so far.

Bushranger Joe Byrne's armour on MRPD at HIFAR in 2003

Rapid Heat Quench Cell for QUOKKA

Prime Minister John Howard at the formal opening of OPAL in 2007

QUOKKA $1m^2$ detector

Terry Noakes and team, at Nepean Engineering with PELICAN's vacuum vessel

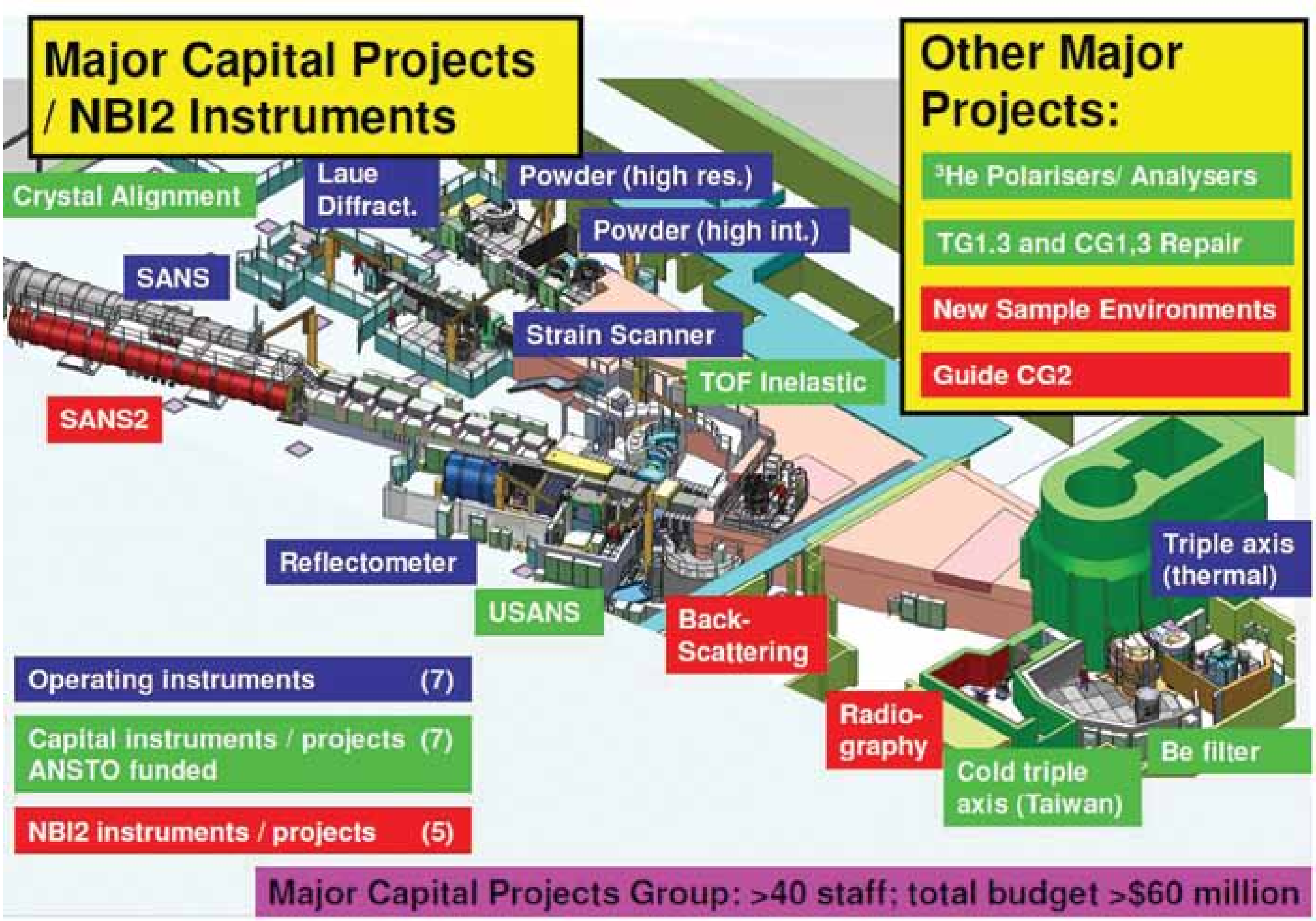
Bragg Institute in 2012

The high life with Mirrotron in Hungary

Workshop on high-field magnets for neutron scattering in Queenstown, New Zealand in 2005

The Neutron Beam Expansion Program (2009-2013)

Frank Klose and Paris Constantine



The great financial crisis hit the world in 2008 and Australia was not immune to these events. With the economy facing a recession, the Government released several economic stimulus packages. Following the onset of this financial crisis, Canberra asked ANSTO to propose possible infrastructure areas where additional funding might be productively allocated. The Bragg Institute acted quickly and proposed, based on earlier requests by its scientific users (e.g. the 2005 Blue Mountains Workshop), a significant *Expansion Plan for Neutron Science in Australia.* The proposal was successful in securing funds and was publicly announced on 12 May 2009 as part of the Super Science – Future Industries initiative. The description of the $37 million project reads as follows: *"This project will significantly enhance the research capabilities of the Australian neutron science facilities at ANSTO. It will provide university, government and industry based users of the new ANSTO research reactor OPAL with new world-class facilities for investigating the structure and dynamics of condensed matter with particular emphasis on the areas nanoscience, soft matter dynamics and biology which are key areas for* *future technology and industrial developments in Australia"*. The Neutron Beam Instruments Expansion Program (NBI2) officially commenced in July 2009 with the goal to build three new instruments, a new cold neutron guide and new world-class sample environments. As always, there was no free lunch. The economic stimulus related funding for NBI2 had the serious constraint of spending the funds within the following four years.

In order to provide the appropriate management structure which could deal with all the existing construction projects (PELICAN, SIKA, KOOKABURRA, JOEY, Be Filter and ^{3}He Project) as well as with these five new NBI2 instruments/projects, the Bragg Institute formed the Major Capital Projects group. The hiring of staff was a major task over the first six months and by 2011 well over forty staff were working for the Major Projects group. Many of them already had experience from the NBI-1 Project.

The NBI2 Scoping Workshop (27-28 August 2009) developed scientific cases and preliminary specifications for the three new NBI2 instruments. These are: a) BILBY, the time-of-flight small-angle neutron scattering instrument; b) DINGO, the radiography/tomography instrument and c) EMU, the backscattering spectrometer. More detailed scientific specifications, schedules and costings were developed during the NBI2 Conceptual Design Workshop (9 November - 4 December 2009) which was hosted by NIST, in the USA. This was also a great team-building activity.

The previous Beam Instruments Advisory Group (BIAG) was reinstated in January 2010 and now reviews the progress of the NBI2/MCP projects on a bi-yearly basis. Successful quarterly progress reports to the government have enabled the necessary release of the required construction funds from the government.

By October 2010, all five NBI2 projects had their instrument proposals approved by the NBI2 Steering Committee. In 2011, most of the detailed designs of instrument components were complete, orders had been placed and detailed engineering designs approved. In 2011 and 2012, major changes to the initial infrastructure of the Bragg Institute were completed, in order to accommodate the new MCP/NBI2 instruments. Major installations of the new instruments started early in 2012 and major changes to the OPAL reactor (insertion of the CG2 guides) were completed in December 2012.

As at the end of 2012, PELICAN, SIKA and JOEY were in the hot-commissioning stage and major components of KOOKABURRA had been installed. Over 2013, these instruments and DINGO will obtain their operational licenses and from there both BILBY and EMU will complete their installation work in order to transition to hot-commissioning and operations in 2014.

This journey has benefited the Australian community in both providing needed employment and scientific infrastructure for further scientific gain and proud engagement of the global community. Steering this progress has developed much cherished technical expertise and leadership. We look forward to further driving the completion of this exciting program for all Australians to embrace.

By October 2010, all five NBI2 projects had their instrument proposals approved

Bragg Institute and the International Atomic Energy Agency

Joseph Bevitt and Herma Büttner

The statute and mandatory responsibilities of the IAEA include supporting its member states in the promotion of peaceful uses of nuclear energy in concert with global nuclear non-proliferation, security and safety objectives. The IAEA has introduced the concept of designating Collaborating Centres to assist in implementing specific areas of its program of research, development and training in nuclear technologies.

IAEA

International Atomic Energy Agency

H.E. Mr. Peter Shannon

Ambassador
Resident Representative of Australia to the
International Atomic Energy Agency
Mattiellistrasse 2-4/111
1040 Vienna

2007-03-14

Subject: Designation of the Australian Nuclear Science and Technology Organisation (ANSTO) as an IAEA Collaborating Centre

Sir,

I have the honour to refer to the discussions between the IAEA Secretariat and Mr. Ian Smith, CEO and Dr. Herma Buttner concerning the designation of ANSTO as an IAEA Collaborating Centre.

You may be aware that the Department of Nuclear Sciences and Applications is, on a three-year trial basis, designating some institutions as IAEA Collaborating Centres. The IAEA Collaborating Centre scheme is similar to those operated by WHO and FAO, which between them have designated over 1,400 such centres worldwide. The concept is that an institution which has worked with the Department in support of its regular budget activities agrees to collaborate formally in accordance with an agreed workplan for a period of three years. In return and in acknowledgement of the contribution, the IAEA designates the institution as an IAEA Collaborating Centre. The IAEA will present the institution with a plaque for public display. The designation does not imply pre-eminence in the specific scientific field, or confer any special honour; rather it is a public recognition of the collaboration with the IAEA in a specific field of work.

We believe that the scheme has good potential to expand our programmatic base, and at the same time extend our collaboration with the many institutions worldwide with which we work to mutual benefit. The formal definition of an IAEA Collaborating Centre is attached as the document entitled "IAEA Collaborating Centres – Concept and Definition". I also attach an explanatory document that we have produced to explain the concept while in the trial stages.

The Department of Nuclear Sciences and Applications has worked closely with ANSTO and we now wish to enhance collaboration in the field of neutron scattering. Our informal exchanges with ANSTO have produced the attached basis for a workplan.

In view of the above, I have the honour to request that the Government of Australia agree to the designation of ANSTO as an IAEA Collaborating Centre.

Accept, Sir, the assurances of my highest consideration.

Werner Burkart
Deputy Director General
Head of the Department of Nuclear Sciences and Applications

Enclosures

cc: Mr. I. Smith
Mr. R. Hutchings

Just in time for the official opening of the OPAL reactor, ANSTO and the Department of Nuclear Sciences and Application of the International Atomic Energy Agency (IAEA) agreed on a work plan for an IAEA Collaborating Centre (see letter above). Subsequently, the IAEA Deputy Director General Werner Burkart announced the collaboration on 20 April 2007, providing ANSTO with its new plaque.

The designation of ANSTO as an IAEA Collaborating Centre for Neutron Scattering Applications recognised the role that OPAL and the state-of-the-art neutron beam facilities of the Bragg Institute have in developing relevant engineering and scientific expertise, whilst also leading to potential improvements in health and nutrition, and the environment.

ANSTO and the IAEA initiated a collaboration and consultation with the view of increasing the neutron-scattering community and promoting neutron scattering in the Asia-Pacific region. A formal work plan was created that emphasised collaboration in the following areas:

- Access to the OPAL neutron-beam facility
- Developing neutron instrumentation
- Promoting applications
- Attracting new users
- Inviting and training scientists, including assistance to the IAEA's training program.

In this context, the development of an 'ambassador' program was envisaged to increase the knowledge about neutron scattering in countries in the Asia-Pacific region. In the long run, such 'ambassadors' will not only increase our user community, but they

Group photo 2007

2007 on KOWARI

Saying ‘thank-you’ on QUOKKA

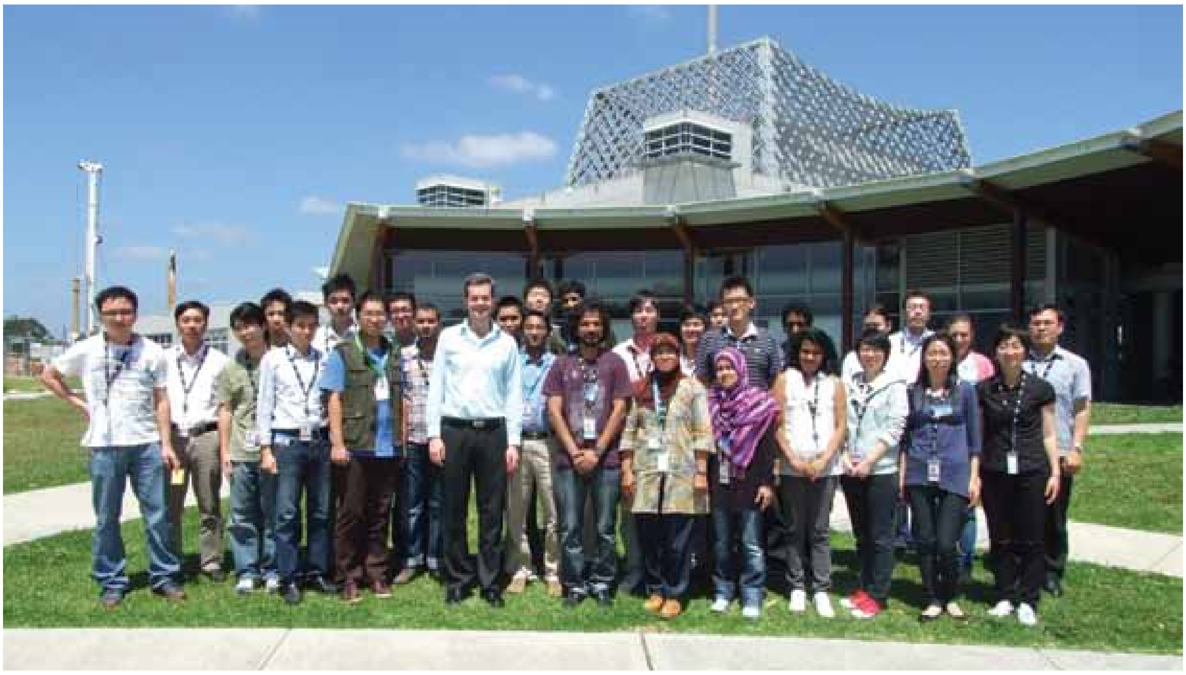
James Hester explaining ECHIDNA

will also contribute to the overall understanding of the use of neutrons for scientific and industrial purposes.

Consequently ANSTO continues to provide assistance to the IAEA’s training and education programs for the neutron user community, organising thematic workshops and schools for students and early career scientists in the use of neutron scattering in particular scientific fields. These workshops include hands-on experiments whilst also encouraging collaboration with universities and research centres.

Our annual neutron school held at the OPAL neutron-beam facility, the ANSTO-AINSE Neutron School on Diffraction, organised in collaboration with the IAEA, was held on 29 November - 3 December 2007. This event was attended by 30 PhD students and postdocs, selected from 55 applicants. Although many of the participants came from Australian universities, together with some from Japan and Taiwan, more than half of the participants originated from other countries including China, Finland, India, Indonesia, Italy, New Zealand, Russia, Ukraine, USA and Vietnam, contributing to a truly international event. The IAEA provided funding for two participants. The school was a great success, with many of the students (both national and international) returning to OPAL to conduct neutron experiments and acting as successful ambassadors at other facilities or universities running their own research programs.

The Institute has since hosted a number of schools, each with its own focus. As a key player in the newly created Asia-Oceania Neutron Scattering Association (AONSA), the Institute has also hosted two international AONSA Neutron Schools. The 4th AONSA Neutron School held in 2011 was originally to be hosted by the Japanese neutron-scattering facilities – the JRR-3M nuclear reactor and J-PARC spallation neutron source. Following the disaster of the Great East Japan Earthquake in March 2011 the Japanese neutron-scattering facilities did not have the ability to train students and the school was cancelled. ANSTO, with the support of AONSA, the Prime Minister’s Education Assistance Program for Japan and AINSE, was honoured to host the 4th AONSA Neutron School, attended by 31 delegates from Australia (8), China (4), India (3), Indonesia (2), Japan (4), Korea (2) and Taiwan (8). The AONSA Neutron Schools have helped attending early-career researchers build expertise and confidence in the application of neutron scattering techniques. We hope that one day these researchers are educating the next generation in the application of neutron scattering.



Above and top, school participants from China, India and Indonesia whose attendance was directly supported by the IAEA.
Top right: an early morning bushwalk.

List of Neutron Schools held at ANSTO:

2007: ANSTO – AINSE Neutron School on Diffraction

2008: ANSTO – AINSE Neutron School on Materials

2009: 2nd AONSA Neutron School

2010: ANSTO – AINSE Neutron School on Dynamics and Kinetics

2011: ANSTO – AINSE Neutron School on Order and Disorder

2011: 4th AONSA Neutron School

2012: Powder Diffraction at Australia's Synchrotron and OPAL Facilities: Experiment Planning to Data Analysis

Due to its success the IAEA Collaborating Centre agreement was extended in 2010 to run another three years.

A vision for the future

Rob Robinson

On 18-19 October 2012, the leadership of the Bragg Institute met with representatives of staff, customers and stakeholders at the Old Quarantine Station in Manly, for a meeting on Strategic Leadership. As part of that meeting, I outlined a possible vision for what the Institute might look like in five years' time in 2017. I started by reflecting that I had arrived at ANSTO in December 1999, just prior to receiving the bids to build what became the OPAL Research Reactor, including a state-of-the-art cold neutron source, supermirror guides, a large modern guide hall and eight neutron beam instruments. The vision was clear - to succeed in the project management and construction of the neutron beam facilities at OPAL, and essentially to build up a new organisation almost from scratch. At the time, the neutron-scattering and synchrotron radiation group in the old ANSTO Physics Division consisted of 17 staff, and while there were excellent and experienced people in the group, it was clear that there was a major opportunity for change and growth. In large measure, that original vision has come to pass, and has indeed been surpassed. I had always thought that I might stay at ANSTO long enough to raise the funding for a second neutron guide hall at OPAL, which together with the first might allow for thirty or more instruments at OPAL. This vision was already intrinsic in the design of OPAL, and is a testament to Shane Kennedy, John White, Helen Garnett and others who had strived for a strong science program for Australia at OPAL. I must admit that I thought that, having raised such funding, responsibility would be passed on to the next generation for implementation, and that I might then be able to retire in peace.

So what is the vision for the Bragg Institute in the next five years?

For a start, we might hope that by 2017 the Bragg Institute and the Australian Synchrotron will be operating 13 instruments each in full user-service mode. We might also have a further three instruments nearing completion, and the final guide (TG2) being installed during the 10-year shutdown of OPAL. Of course, during the same shutdown, we would be replacing the in-pile guide components on four out of five of OPAL's shutters and changing out the cold neutron source. One would hope that improvements in design and performance of OPAL's first cold source would be implemented.

Of course, the whole Institute and the National Deuteration Facility will have been housed in the same building complex for several years. Funding might have been lined up for the Second Guide Hall, with up to ten end-guide positions and eight initial neutron beam instruments. In addition, there will be funding commitments to build additional instruments from other governments in the Asia-Pacific region.

The existing operational program at OPAL, might be bringing in as much as $500,000 in commercial revenue, particularly for strain scanning, radiography and imaging, small-angle scattering and with modest contributions from all other instruments. We might hope that thirty or so commercial companies might be using us in any given year, including some big-name multinationals. We should not rule out the possibility a beam line dedicated to the interests of the National Health and Medical Research Council, much as the US National Institutes of Health have funded similar activities at NIST. Likewise we might envisage having CSIRO staff based permanently at OPAL to service that organisation's needs, and indeed ANSTO's own Institute of Materials Engineering might also do this.

What is the vision for the Bragg Institute in the next five years?

Transport, food and lodging remain key issues for our users and we would hope that there is new lodging across the parking lot from the Neutron Guide Hall, within walking distance, as is common at overseas neutron facilities, and at the Australian Synchrotron.

Regarding ANSTO's own research drivers (as opposed to those of our users and partners), we would hope to maintain our leadership position in food science, Li-ion batteries and other energy materials, in engineering materials and in deuterated materials. In addition, we might hope to start two new areas that would 'take off' in the meantime. Of course, there should be closer integration of modelling with the


OPAL's neutron guide hall 2011


OPAL in 2012


Showing Senator Chris Evans around in 2012

neutron experiments, with everything from electronic structure and molecular dynamics up to finite-element modelling for materials engineering.

We will have a strong enough team that some of our alumni will hold down chairs in leading universities, and others will be running other major facilities elsewhere. It would be good to have a cadre of thirty or so postdoctoral fellows based in the Institute, some of them possibly funded jointly with the Australian Synchrotron.

We would hope to be producing a steady stream of articles in the highest-profile general-interest scientific journals, and indeed that OPAL is known internationally for one or more really big things. We might also aspire to have some genuine development activities, of components or devices that we need for our program at OPAL, that could be spun-off into a small company local to ANSTO.

Finally, regarding culture, we should be realistic that we might still have the sort of creative tension that exists in all hotbeds of innovation. Of course we would hope to avoid the destructive behaviours that sometimes crop up in such environments, but we do not want to snuff out the essence of creativity that sometimes comes from a modest amount of ferment.

Timeline

2002

14 October 2002: Announcement to staff of break-up of ANSTO's Physics Division, and formation of the Bragg Institute

1 December 2002: Bragg Institute formed

2003

19 March 2003: The Bragg Day Out, at Como Hotel

31 March 2003: Inaugural meeting of Bragg Institute Advisory Committee

3 July 2003: Measurements on bushranger Joe Byrne's armour, on MRPD at HIFAR

21 November 2003: 1st neutron reflectivity profile at ANSTO at HIFAR

2004

23 February 2004: HIFAR 3-Axis Spectrometer converted into a strain scanner

1 July 2004: ANSTO decides to invest $5M in the Australian Synchrotron

17 July 2004: Jill Trewhella wins Federation Fellowship with Sydney University and ANSTO

19 August 2004: Decision to build IN6-style time-of-flight instrument (PELICAN) as the 8th instrument at OPAL

1 September 2004: Peer Review introduced for all neutron scattering experiments at HIFAR, including ANSTO's work

10 December 2004: X-Ray Reflectometer installed in B82

2005

8 June 2005: Agreement signed with National Science Council of Taiwan to construct SIKA cold-neutron 3-Axis Spectrometer

27 November – 2 December 2005: ICNS 2005 Conference

2-4 December 2005: Blue Mountains Workshop

2006

31 March – 3 April 2006: Move into B87 (Bragg Institute Building)

12 August 2006: OPAL criticality

27 November 2006: NCRIS Funding for National Deuteration Facility Announced

18 December 2006: First Neutron Diffraction Pattern from OPAL (from ECHIDNA)

2007

30 January 2007: Minister Julie Bishop shuts down HIFAR

20 April 2007: Prime Minister John Howard opens the OPAL reactor

19 October 2007: First paper from OPAL

Appendix 1 - Timeline

2008

7 March 2008: Formation of AONSA

2 July 2008: First Single-Crystal Structure Refinement from OPAL

4 September 2008: First SANS pattern from OPAL

2009

23 January 2009: Contract signed with ILL for ^{3}He Polariser System

19 February 2009: First phonon measurement at OPAL

13 May 2009: Budget announcement of $37M for new cold guides and 3 new instruments for OPAL

1 July 2009: Merger of National Deuteration Facility into Bragg Institute

17 July 2009: Launch of Mail-in Service on ECHIDNA

7 September 2009: First joint paper between Australian Synchrotron and OPAL

9 October 2009: Inauguration of Sutherland-ANSTO shuttle-bus service for users

2010

2 February 2010: First experiment at OPAL using deuterated material from the National Deuteration Facility

11 March 2010: NBI-2 Team moves into Hut-77

30 June 2010: Bragg Institute extension approved

31 August 2010: 50 papers from OPAL

28 September 2010: First paper from QUOKKA

2011

4 January 2011: First *Phys. Rev. Letter* from OPAL

23 March 2011: Move to fixed proposal deadlines at OPAL

9 May 2011: Helping our Japanese friends following the Great Tohoku Earthquake

10 July 2011: 100 Papers from OPAL

20 November 2011: First Asia-Oceania conference on Neutron Scattering, in Tsukuba, Japan

9 December 2011: First Neutrons into PELICAN

2012

30 March 2012: First *Science* article from OPAL

16-18 April 2012: Workshop on second guide hall for OPAL

21 August 2012: 200 research papers from OPAL

6 October 2012: First neutrons into SIKA

Bragg Institute Advisory Committee

Chairs:

Don Napper	(Sydney University)	2003 - 2007
John White	(Australian National University)	2008 - 2010
Peter Colman	(Walter and Eliza Hall Institute)	2011 - 2013

Members:

Don Napper	(Sydney University)	March 2003 – April 2007
George Collins	(ANSTO-Materials)	March 2003 - April 2006
Evan Gray	(Griffith University)	March 2003 - April 2004
Rob Lamb	(UNSW)	March 2003 – April 2004
Alan Leadbetter	(Exeter University, UK)	March 2003 - April 2007
Barrie Muddle	(Monash University)	March 2003 - April 2007
Brian O'Connor	(Curtin University)	March 2003 – April 2008
Yasuhiko Fujii	(University of Tokyo, Japan)	March 2003 – April 2008
Mike Rowe	(NIST, USA)	September 2003 – April 2009
John White	(Australian National University)	October 2004 – May 2010
Rob Burford	(UNSW)	April 2005 – April 2009
Lyndon Edwards	(ANSTO-Materials)	April 2007 – present
Bill Stirling	(ESRF, France)	April 2007 – April 2013
Keith Nugent	(University of Melbourne)	April 2008 - present
Masa Arai	(J-PARC, Japan)	April 2009 - present
Peter Colman	(Walter and Eliza Hall Institute)	April 2009 - present
Kurt Clausen	(Paul Scherrer Institute, Switzerland)	May 2010 - present
Jill Trewhella	(Sydney University)	May 2010 – present
Cathy Foley	(CSIRO)	April 2012 – present

Beam Instruments Advisory Group (2000-2007 and 2009-2013)

Chairs:

Tony Klein	(University of Melbourne)	2000 - 2007
Dan Neumann	(NIST, USA)	2009 - 2013

Members:

Tony Klein	(University of Melbourne)	December 2000 – February 2007
Yasuhiko Fujii	(University of Tokyo, Japan)	December 2000 – February 2003
Evan Gray	(Griffith University)	December 2000 - February 2003
Gerald Roach	(Alcoa)	December 2000 - February 2007
Sunil Sinha	(University of California San Diego, USA)	December 2000 - February 2003
Lou Vance	(ANSTO-Materials)	December 2000 – July 2004
John White	(Australian National University)	December 2000 – July 2004
Brendan Kennedy	(Sydney University)	December 2000 – July 2002
Ian Gentle	(University of Queensland)	July 2001 – February 2013
Rod Hill	(CSIRO)	July 2001 – February 2003
Michi Furusaka	(University of Hokkaido, Japan)	August 2003 - February 2013
Dan Neumann	(NIST, USA)	August 2003 - February 2013
Garry Seaborne	(Major Projects Victoria)	August 2003 – February 2005
Stewart Campbell	(Australian Defence Force Academy)	February 2004 – February 2007
Kath Smith	(ANSTO-Materials)	February 2005 - February 2007
John Dunlop	(CSIRO)	July 2005 - February 2007
Don Kearley	(Technical University Delft, Netherlands)	July 2006
Sow-Hsin Chen	(Massachusetts Institute of Technology, USA)	February 2007
Ken Anderson	(European Spallation Source, Sweden)	February 2010 - February 2013
Craig Buckley	(Curtin University)	February 2010 - February 2013
Greg Warr	(Sydney University)	February 2010 - February 2013
Steve Wilkins	(CSIRO)	February 2010 - February 2013
Eberhard Lehmann	(Paul Scherrer Institute, Switzerland)	July 2010 - February 2013

Program Advisory Committee

Chairs:

Jill Trewhella	(Sydney University)	2007 - 2008
Calum Drummond	(CSIRO)	2009 - 2010
Anton Middelberg	(University of Queensland)	2010 - present

ANSTO Non-voting Secretary:

Herma Büttner:		July 2007 - July 2009
Joseph Bevitt:		February 2010 - present

Members:

Jill Trewhella	(Sydney University)	July 2007 – December 2008
Craig Buckley	(Curtin University)	July 2007 – December 2008
Stewart Campbell	(Australian Defence Force Academy)	July 2007 – December 2008
Calum Drummond	(CSIRO)	July 2007 – February 2010
Hugh O'Neill	(Australian National University)	July 2007 – February 2010
Huan-Chiu Ku	(National Tsing Hua University, Taiwan)	July 2007 – December 2008
Ward Beyermann	(University of California Riverside, USA)	December 2008 – August 2011
Valerie Linton	(University of Adelaide)	December 2008 – February 2010
Rob Burford	(UNSW)	July 2009 - present
Cheng-Hsuang Chen	(National Taiwan University, Taiwan)	July 2009 - February 2011
Paul Curmi	(UNSW)	July 2009 - present
Brendan Kennedy	(Sydney University)	July 2009 - present
Anton Middelberg	(University of Queensland)	July 2009 – present
Mau-Tsu Tang	(NSRRC, Taiwan)	February 2010
Duncan McGillivray	(University of Auckland, New Zealand)	February 2010
George Collins	(CAST-CRC)	July 2010 - present
Andrew Whitten	(University of Queensland)	July 2010
Chris Ling	(Sydney University)	July 2010 – May 2012
Allan Pring	(South Australian Museum)	July 2010
Ian Jackson	(Australian National University)	February 2010 – November 2011
Keng Liang	(National Chiao Tung University, Taiwan)	August 2011
Frank Bruhn	(AINSE)	November 2011
Evan Gray	(Griffith University)	November 2011
An-Chung Su	(National Science Council, Taiwan)	November 2011
Oleg Sushkov	(UNSW)	November 2011
Chung-Yuan Mou	(National Taiwan University, Taiwan)	May 2012
Tracy Rushmer	(Macquarie University)	May 2012 - present
Robert Knott	(ANSTO)	May 2012
Hsiung Chou	(National Sun Yat-Sen University, Taiwan)	November 2012
Rob McQueeney	(Iowa State University, USA)	November 2012 - present

Theses containing data from Bragg Institute facilities (2002-2012)

PhD:

1. D. Losic, The exploitation of self-assembled monolayers for the fabrication of enzyme biosensors, Flinders University, 2002.
2. Daniel Riley, Self-propagating high-temperature synthesis of Ti_3SiC_2, Newcastle University, 2002 (from MRPD).
3. Jenny Forrester, In-situ diffraction study of perturbed ferroelectric crystal structures, Newcastle University, 2002 (from MRPD and HRPD).
4. Vanessa K. Peterson, Diffraction investigations of cement clinker and tricalcium silicate using Rietveld analysis, University of Technology Sydney, 2003, (from MRPD and HRPD)
5. Kia S. Wallwork, *Ab initio* structure determination of minerals and inorganic materials by powder diffraction methods, School of Chemistry, Flinders University, 2003 (from HRPD)
6. Joan Conolly, Development of Biomedical Applications of Magnetic Fluids and Investigation of Their Physical Properties, 2003, University of Western Australia (from AUSANS)
7. Rene Macquart, Structural studies of ferroelectric oxides, School of Chemistry, University of Sydney, 2003 (from HRPD).
8. Namita R. Choudhury, Structure–rheology relationship in viscosity index improver, Ian Wark Research Institute, University of South Australia, 2003 (from AUSANS)
9. S. Pratapa, Diffraction-based modelling of microstructural size and strain effects in sintered ceramics, Applied Physics, Curtin University of Technology, 2003 (from HRPD)
10. Martin G. Markotsis, Preparation and characterisation of TPE IPNs using radiation methods, School of Chemical Engineering and Industrial Chemistry, University of New South Wales, 2003 (from AUSANS).
11. Chris J. Garvey, A study of the hydration of paper sheets, School of Chemical Engineering, Monash University, 2003 (from AUSANS)
12. Enny Silviani, Cation effects on the catalytic activity of the $[PMo_{12}O_{40}]^3$ ion in the oxidative dehydrogenation of isobutyraldehyde, School of Environmental and Life Sciences, University of Newcastle, 2003 (from MRPD)
13. Nigel Kirby, Barium zirconate ceramics for melt processing of barium curprate superconductors, Department of Applied Physics, Curtin University of Technology, 2004 (from MRPD)
14. Gianluca Paglia, Determination of the structure of γ-alumina using empirical and first principles calculations combined with supporting experiments, Department of Applied Physics, Curtin University of Technology, 2004 (from MRPD and HRPD)
15. Kirily Rule, Magnetic ordering in the two dimensional antiferromagnet, $FePS_3$, School of Physics and Material Engineering, 2004 (from Longpol and MRPD)
16. Matthew R. Rowles, The structural nature of alumimosilicate inorganic polymers: a macro to nanoscale study, Curtin University of Technology, Department of Applied Physics, 2004 (from MRPD)
17. Mark Pitt, In-situ powder diffraction studies of metal hydrogen microstructures, School of Science, Griffith University, 2004 (from MRPD)
18. Frank J. Brink, Oxygen/fluorine ordering, modulated structures and solid state solutions in metal oxyfluoride systems, Research School of Chemistry, Australian National University, 2004 (from HRPD).
19. Annabelle Blom, Structure and physical properties of surfactant and mixed surfactant films at the solid-liquid interface, School of Chemistry, University of Sydney, 2005 (from neutron reflectometer)
20. Andrew E. Whitten, Electrical and optical properties of molecules in crystals, University of New England, 2005 (from 2TANA)
21. Keith G. McLennan, Structural Studies of the Palladium-hydrogen System, School of Science Griffith University, 2005 (from MRPD)
22. Joseph Bevitt, Functionalised Nanoporous Molecular Materials, School of Chemistry, University of Sydney, 2006 (from 2tanA)
23. Valeska P. Ting, Structural studies of the photocatalytic A_2InNbO_6 and $A_3CoNb_2O_9$ (A = Ba, Sr and Ca) compounds, Research School of Chemistry, Australian National University, 2006 (from HRPD)
24. Lisa E. Rodgers, The molecular characterisation of sol-gel biocatalysts, School of Biotechnology and Biomolecular Sciences, University of New South Wales, 2006 (from AUSANS and SAXS).
25. Catherine Kealley, Synthesis and characterisation of carbon nanotube reinforced hydroxyapatite ceramics for biomedical applications, University of Technology Sydney, 2006 (from HRPD)
26. John Daniels, Relaxation and Microstructural Studies in Ferroelectrics, School of Physics and Material Engineering, Monash University 2007 (from TASS)
27. Nathan A. S. Webster, New fluorite-type Bi_2O_3-based solid electrolytes: characterisation, conductivity and crystallography, School of Biomedical and Chemical Sciences, University of Western Australia, 2007 (from HRPD)
28. Jennifer L. Lowe, DSP in the Bayer process : a fundamental study of its precipitation and role in impurity removal, Department of Applied Chemistry, Curtin University of Technology, 2007 (MRPD)
29. Paul J. Saines, Structural studies of lanthanide double perovskites, School of Chemistry, University of Sydney, 2008 (from HRPD, MRPD, ECHIDNA)
30. Ania M. Ziara-Paradowska, Investigation of Residual Stress in Welds: Using Neutron and Synchrotron Diffraction, Department of Mechanical Engineering, Monash University 2008 (from TASS)
31. Thomas Lenné, The effects of solutes on the phase behaviour of phospholipid membranes, School of Applied Sciences, RMIT University, 2008 (from AUSANS)
32. Tri-Hung Nguyen, Investigation of novel liquid crystalline materials for the sustained oral delivery of poorly water soluble drugs, Faculty of Pharmacy and Pharmaceutical Sciences, Monash University, 2008 (from SAXS)
33. Geoffrey C. F. Johnston-Hall, New insights into diffusion-controlled bimolecular termination using ‘controlled/living’ radical polymerisation, School of Chemistry and Molecular Bioscience, University of Queensland, 2008 (from SAXS)
34. Neeraj Sharma, Synthesis, structure and properties of some novel transition metal-doped bismuth oxides : from fluorite-type to aurivillius-type, School of Chemistry, University of Sydney, 2009 (from Koala, HRPD and MRPD)
35. Peter George, Engineered Surfaces for Biomaterials and Tissue Engineering, Australian Institute for Bioengineering and Nanotechnology, University of Queensland, 2009 (from X-ray reflectometer)

36. Simone Ciampi, A versatile and modular approach to modify silicon surfaces for electrochemical applications, School of Chemistry, University of New South Wales, 2009 (from X-ray reflectometer)

37. Tanja Kjallman, Surface-immobilized hairpin DNA sensors for direct and specific detection of target DNA, School of Chemical Sciences, University of Auckland 2009. (from PLATYPUS, X-ray reflectometer)

38. Yao Da Dong. Investigation of nanostructured liquid crystal particles as novel agrochemical delivery agents, Faculty of Pharmacy and Pharmaceutical Sciences, Monash University, 2009 (from SAXS)

39. Abhijit Pramanick, On the correlation of dynamic electric-field induced structural changes and piezoelectricity in ferroelectric ceramics, University of Florida 2009 (from WOMBAT)

40. Mark Paskevicius, A nanostructural investigation of mechanochemically synthesised hydrogen storage materials, Department of Imaging and Applied Physics, Curtin University of Technology, 2009 (from WOMBAT)

41. Betime Nihiji, Structure and properties of epoxy nanocomposites Institute for Technology Research and Innovation, Deakin University, 2009 (from SAXS)

42. Gordon Thorogood, Structure and Properties of Metal Oxides for Use in Cation Exchange, University of Sydney, School of Chemistry, PhD in Inorganic Chemistry, 2009 (from WOMBAT and ECHIDNA)

43. Matthew R. J. Carroll, The effects of polymer coatings on the proton transverse relaxivities of superparamagnetic nanoparticle MRI contrast agents, School of Physics, University of Western Australia, 2010 (from SAXS)

44. Jean-Pierre Veder, The Development of a Rigorous Nanocharacterisation Scheme for Electrochemical Systems, Nanochemistry Research Institute, Curtin University of Technology, 2010 (from PLATYPUS, X-ray reflectometer)

45. Nobuo Tezuka, Microstructural design of mullite-based ceramics from clay minerals, Curtin University, 2010. (from WOMBAT)

46. Pang, WK, Thermal and Phase Stability of Novel Layered Ceramics – $M_{n+1}AX_n$ Phases, Curtin University, 2010 (from ECHIDNA, WOMBAT)

47. SM Knupfer, Iterative laser straightening of welded plates of varying thickness, Heriot-Watt University (2010) (from KOWARI)

48. Rashmi Nigam, Study of Magnetic Behaviour in Ru-based Superconducting Ferromagnets, Institute for Superconducting and Electronic Materials, University of Wollongong, 2010 (from WOMBAT)

49. Nishar Hameed, Self-assembled diblock copolymer complexes via competitive hydrogen bonding, Institute for Technology Research and Innovation, Deakin University, 2010 (from SAXS)

50. Luke Ryves, Deposition of nanostructured thin films using a high current pulsed arc, School of Physics, University of Sydney, 2010 (from X-ray reflectometer)

51. Andrew M. Telford, Advanced functional coatings for biomedical applications: patterning cells onto biomaterials, School of Chemistry, The University of Sydney, 2011. (from PLATYPUS, X-ray reflectometer)

52. Arthur R. G. Smith, Properties of Materials for Organic Light Emitting Diodes, School of Chemistry and Molecular Bioscience, University of Queensland, 2011 (from NDF - Chemical Deuteration, PLATYPUS, X-ray reflectometer)

53. Bin Guan, Fabrication of porous silicon photonic crystal microparticles: towards single cell sensing, School of Chemistry, University of New South Wales, 2011 (from X-ray reflectometer)

54. Donna Jade Menzies, The generation and characterisation of low fouling, uniform, gradient and micropatterned surfaces via plasma polymerisation, Department of Materials Engineering, Monash University, 2011 (from PLATYPUS)

55. Elizabeth A. Fellows, Synergistic interplay between spin crossover and host-guest function in a family of coordination framework materials, School of Chemistry, The University of Sydney, 2011. (from ECHIDNA, WOMBAT)

56. Hamish Cavaye, Dendrimer sensors for explosives, School of Chemistry and Molecular Biosciences, University of Queensland, 2011 (from NDF - Chemical Deuteration, PLATYPUS, X-ray reflectometer)

57. Jimmy Ting, Crystal Structure and physical properties of Aurivillius phases and perovskites, School of Chemistry, The University of Sydney, 2011 (from ECHIDNA)

58. John Chow, Conformational Responses of proteins to Complex Formation and Molecular Crowding, School of Molecular and Microbial Biosciences, The University of Sydney, 2011 (from Bruker (SAXS), NDF - Biodeuteration, QUOKKA)

59. Kateryna Bazaka, Fabrication and characterization of plasma polymer thin films from monoterpene alcohols for applications in organic electronics and biotechnology, School of Engineering and Physical Sciences, James Cook University, 2011 (from X-ray reflectometer)

60. Richard Clements, Structure and Bonding in Lanthanide Zirconates, School of Chemistry, The University of Sydney, 2011. (from ECHIDNA)

61. Samuel G. Duyker, Lanthanoid Coordination Framework Materials: Thermal Expansion, Host-Guest and Electrochemical Properties, School of Chemistry, The University of Sydney, 2011. (from Computing Cluster, Koala, WOMBAT)

62. Sarah D. Pretty, Investigating Interfacial Reactions of Silver Containing Films Using Novel Methods, Department of Chemistry, The University of Western Ontario, London, Ontario, Canada, 2011 (from PLATYPUS)

63. Maggie Chai Cin Ng, Design characteristics of metal organic frameworks: from rigidity to flexibility, University of New South Wales, 2011 (from WOMBAT).

64. Cheuk Chi Albert Ng, Switchable surfaces for cell biology, School of Chemistry, University of New South Wales, 2011 (from X-ray reflectometer)

65. Ben Kent, Location of sugars in bilayer and non-bilayer lipid phases: relevance to membrane preservation during desiccation, School of Applied Sciences, RMIT University, 2011 (from X-ray reflectometer, QUOKKA)

66. Nisha Aravind, "Development and Evaluation of Functional Food pasta", University of New England, 2011 (from SAXS)

67. Sunil K. Karna, Spin, charge and lattice couplings in layered oxychalcogenide BiOCuX (X= S, Se) compounds studied by neutron diffraction, Department of Physics, National Central University, Taiwan, 2011 (from ECHIDNA)

68. Ryan D. Mills, Biochemical and biophysical analysis of enzymatic domains of the Parkinson's disease-causative protein leucine-rich repeat kinase (LRRK2), Department of Biochemistry and Molecular Biology, Department of Pathology, Bio21 Molecular Science and Biotechnology Institute, University of Melbourne, 2011 (from SAXS)

69. David A. Jacques Histidine kinase regulation by protein inhibitors, School of Molecular and Microbial Biosciences, University of Sydney, 2011 (from SAXS)

70. Jason Alexander Schiemer, Average and local structure, phase transitions and physical properties of key lead-free ferroelectric materials, Australian National University, 2012 (from WOMBAT)

71. Matthew Griffith, Charge Generation and Recombination in Porphyrin Based Dye Sensitized Solar Cells, Intelligent Polymer Research Institute, University of Wollongong, 2012 (from X-ray reflectometer)

72. Mirjana Dimitrijev-Dwyer, Properties of novel biosurfactants: linking the molecular, meso- and macro-length scales, Australian Institute for Bioengineering and Nanotechnology, University of Queensland, 2012 (from NDF - Biodeuteration, PLATYPUS, X-ray reflectometer)

73. Thomas Saerbeck, Magnetic Coupling Phenomena in Systems with Reduced Dimensionality studied with Polarized Neutron Reflectometry, School of Physics, University of Western Australia, 2012 (from PLATYPUS, QUOKKA, TAIPAN, WOMBAT, X-ray reflectometer)

74. Chi-Yen Li, Intrinsic surface and core magnetic moments in Au nanoparticles - neutron diffraction and magnetization studies, Department of Physics, National Central University, Taiwan 2012 (from WOMBAT).

75. Jessica J. Chadbourne, Structures and Properties of Coordination Polymers Containing Tetracyanidometallate Units, School of Chemistry, The University of Sydney, 2012. (from ECHIDNA, WOMBAT)

76. Yue Wu, Understanding and Controlling Anomalous Thermal Expansion Behaviour in Coordination Framework Materials, School of Chemistry, The University of Sydney, 2012. (from ECHIDNA, and Chemical Deuteration)

77. David Fernandez, Membrane Interactions of Australian Antimicrobial Peptides, School of Chemistry, University of Melbourne, 2012. (from NDF - Chemical Deuteration, PLATYPUS)

78. Andrew James Princep, Characterisation of Electronic Multipoles in Rare-Earth Intermetallic Compounds, Department of Physical, Environmental and Mathematical Sciences, University of New South Wales, Canberra Campus, 2012 (from WOMBAT).

79. Po-Wei Yang, Neutron and synchrotron X-ray scattering studies on the structure and phase behavior of mixed short-chain/long-chain bicelles and their interaction with DNA, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan, 2012 (from PLATYPUS, and QUOKKA).

80. Chendur Palaniappan, The effects of cholesterol and cholesterol esters on the interaction of human tear proteins with meibomian lipids, School of Science and Health, University of Western Sydney, 2012 (from X-ray reflectometer).

81. Shiwani Raju, Interfacial viscoelasticity of human meibomian lipid films, School of Science and Health, University of Western Sydney, 2012 (from X-ray reflectometer).

Masters

1. Daehyun Hong, Surface Binding Kinetics of Cell Penetrating Peptides onto Phospholipid Monolayers, Department of Chemistry, Sogang University, Seoul, Korea, 2009 (from PLATYPUS and X-ray reflectometer)

2. I-Ting Liu, Adsorption of DNA by charged diblockcopolymer and lipid monolayer at the air-water interface by Langmuir-Blodgett method and X-ray/neutron reflectivity, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan, 2010 (from PLATYPUS, QUOKKA).

3. Ning-Chun Chi, The Effects of Oxidative Stress on Cellular Membranes, Masters of Science in Chemistry, School of Chemical Sciences, University of Auckland, New Zealand, 2011 (from Bruker (SAXS), PLATYPUS, QUOKKA, X-ray reflectometer)

4. Eric Rey, Investigations on Transition Metal doped Cu_5SbO_6, A thesis submitted in partial fulfilment of the requirements for the degree of Master of Science in Chemistry, The University of Auckland, 2011 (from ECHIDNA)

5. Yi-Wen Ting, Microstructures and magnetic properties of ferromagnetic / antiferromagnetic thin films, Master of Science, Department of Materials Science and Engineering, National Chung Hsing University, Taiwan 2011 (from PLATYPUS, WOMBAT, TAIPAN, and X-ray reflectometer).

6. Say Kwang Lim, Covalent Protein Immobilisation and Patterning on Thin Polymer Films, Masters of Science, School of Chemistry. University of Sydney, 2012 (from PLATYPUS, X-ray reflectometer)

7. Pei-Shi Chen, The influence of ion-beam bombardment and antiferromagnetic layer thicknesses of magnetic thin films, Master of Science, Department of Materials Science and Engineering, National Chung Hsing University, Taiwan 2012 (from PLATYPUS and X-ray reflectometer).

Honours

1. S. Keough, Grazing incidence x-ray studies of lumogen thin films, Flinders University, 2005, (from X-ray reflectometer)

2. Paul J. Saines, Studies of lanthanide doped alkaline earth aluminates and gallates, School of Chemistry, University of Sydney, 2004 (from HRPD)

3. Stewart Pullen, Temperature Jump Cell for SANS instrument, Bachelor of Industrial Design Engineering, 2006 University of Western Sydney, (from QUOKKA)

4. John Chow, The structure of surface-bound tropoelastin and synthetic elastin films, School of Electrical and Information Engineering, University of Sydney, 2006 (from X-ray reflectometer)

5. Benjamin J. Beccari, Structure and magnetism in the reduced layered compound $Nd_{2-x}Sr_xCoO_{4-\delta}$, School of Physics, University of Wollongong, 2006 (from HRPD)

6. Melinda C. L. Cheah, Structural studies of A-site substitutions in double perovskites, School of Chemistry, University of Sydney (2006) (from HRPD)

7. David. A. Jacques, Investigation of the structural basis for the inhibition of histidine kinase A by Sda in Bacillus subtilis, School of Molecular and Microbial Biosciences, University of Sydney, 2006 (from SAXS)

8. Kleydish J, Near-surface structure of cationic surfactants, School of Chemistry, University of Sydney 2005 (from SAXS and HIFAR Reflectometer)

9. Bobillier S Surfactant self-assembly in some ionic liquids, School of Chemistry, University of Sydney, 2005 (from SAXS)

10. Stephen Dekker, Analysis of the density, structure and protein binding properties of plasma modified thin polystyrene films using X-ray reflectometry, School of Physics, University of Sydney, 2007 (from X-ray reflectometer)

11. Jessica M. Hudspeth, The Structure and Magnetic Properties of Rare-Earth Calcium Ferrates, Physics, Australian National University, 2008. (from WOMBAT)

12. Ross Whitfield, Study of phase formation in metal injection moulding through in situ neutron diffraction, Physics, Australian National University, 2008 (from WOMBAT)

13. Rachael Barnett, Characteristics of bio-membranes for implantable bionic devices, 2008, Bachelor of Science (Physics), School of Engineering and Physical Sciences, James Cook University (from X-ray reflectometer)

14. William R. Brant, (2009). Development of Defect Perovskites for use as Cathode Materials in Lithium Ion Batteries. School of Chemistry, The University of Sydney. (from ECHIDNA)

15. Sven. O Sylvester, Solid state photochromic molecular assemblies, School of Chemistry, University of New South Wales, 2009 (from X-ray reflectometer)

16. Ipshita Mandal, Effective protection against bacterial biofilm formation: Surface-immobilisation of antimicrobial protein Hydramacin-1, School of Chemical Sciences, University of Auckland, New Zealand, 2010 (from PLATYPUS, QUOKKA, X-ray reflectometer)

17. Catriona Vanston, Neutron Techniques to Probe Hydride Ligand Fluxionality, School of Chemistry, University of Tasmania, 2011 (from Koala, and NDF – Chemical deuteration)

18. Emily Reynolds, Pyrochlore-Fluorite Transformation in Zirconates, School of Chemistry, The University of Sydney, 2011. (from ECHIDNA, WOMBAT)

19. Peter Akers, Biofilm Prevention using Immobilised Antimicrobial Proteins, School of Chemical Sciences, University of Auckland, New Zealand, 2011 (from PLATYPUS, X-ray reflectometer)

20. Tomas Mayfield, Mimicking the Outer Membrane of Gram Negative Bacteria, School of Medicine, Flinders University, 2011 (from PLATYPUS, X-ray reflectometer)

21. Whittle, T. Honours Thesis, School of Chemistry, The University of Sydney, 2011. (from ECHIDNA)

22. Tjiadarma, D. Honours Thesis, Structure and Property Investigation of Spinel Type $LiMnTiO_4$, School of Chemistry, University of Sydney, 2011. (from ECHIDNA)

23. Lachlan S. F. Henderson, Synthesis and Characterisation of Rare-Earth Oxides, Thesis submitted in part fulfillment of the degree of Bachelor of Engineering, Department of Engineering, Australian National University, 2011. (from ECHIDNA)

24. Sam Brazier-Hollins, Magnetic and Structural Characterisation of Metal Phosphorus Chalcogenides, Bachelor of Engineering Hons, Australian National University 2011. (from ECHIDNA)

25. Kristian Tangso, Investigation of Spiropyran Derivatives as Light Responsive Liquid Crystalline Components, 2011, Monash University. (from NDF-Chemical deuteration)

26. Josie E. Auckett, Influence of oxygen defects on structure, magnetism and ionic conduction in alkali earth ferrites, 2011, School of Chemistry, the University of Sydney (from WOMBAT, Koala, and ECHIDNA)

27. T. Godfrey, Investigation of the Prussian blue analogues $A(III)[B(III)(CN)_6]$ as cathode materials for rechargeable batteries, School of Chemistry, University of Sydney, 2012.

28. Jesse Gabrielle, The physicochemical properties of (O-Acyl)-ω-hydroxy fatty acids and their role in meibomian lipids, School of Science and Health, University of Western Sydney, 2012 (from X-ray reflectometer).

29. Nurafini Assila Mohd Rafi, Phase transitions in the Myverol/saline system induced by fluoro-penetratin, School of Applied Sciences, RMIT University, Melbourne, 2012 (from X-ray reflectometry).

Publications (2002-2012)

2002

1. A. J. Berry and M. James, Refinement of Hydrogen Positions in natural F-Chondrodite by Powder Neutron Diffraction", Mineralogical Magazine 66, 441-449 (2002).
2. R. Cameron, K. Horlock and R. A. Robinson, The Australian Replacement Research Reactor, in proceedings of 13th Pacific Basin Nuclear Conference, PBNC13, Shenzen, China, 21-25 October 2002.
3. S. L. Cram, G. M. Spinks, G. G. Wallace and H. R. Brown, Mechanism of electropolymerisation of methyl methacrylate and glycidyl acrylate on stainless steel. Electrochimica Acta, 47(12), 1935-1948, (2002).
4. L. D. Cussen, Resolution of Neutron Three-Axis Spectrometers by Phase Space Methods, J. Appl. Cryst. 35, 615-623 (2002).
5. L. D. Cussen, A Description of Beams from Focussing Monochromators using Acceptance Diagrams, J. Appl. Cryst. 35, 702-712 (2002).
6. L. D. Cussen, Beam Centre Shifts Caused by Vertical Focussing, Proceedings of SPIE 4785, 83-90 (2002).
7. L. D. Cussen, Resolution of Three-Axis Spectrometers by Phase Space Methods, Applied Physics Letters A, Appl Phys A, 74 [Suppl1], s58-s60 (2002).
8. L. D. Cussen and D. J. Goossens, The influence of background on neutron polariser optimisation, Applied Physics Letters A, 74 [Suppl1], s104-s106 (2002).
9. L. D. Cussen and D. J. Goossens, Optimising Polarised Neutron Scattering Experiments - XYZ and Polarimetry Analysis, Nuclear Instrum. Meth. A 491, 226-232 (2002).
10. L. D. Cussen, E. M.Gray, A. P. Murani, S. J. Kennedy and B. A. Hunter, Long-range atomic order in irradiated $Cu_{80}Mn_{20}$, Europhysics Letters 58, 243-249 (2002).
11. E. Drabarek, J. R. Bartlett, H. J. M. Hanley, J. L. Woolfrey and C. D. Muzny, Effect of Processing Variables on the Structural Evolution of Silica Gels, Int. Journal of Thermophysics, 23, 145-160 (2002).
12. T. Ersez, Bond-Angle Independent Magnetic Interaction in Rhombohedral $La_{0.875}Sr_{0.125}MnO_{3+d}$, Materials Letters 54, 211-216 (2002).
13. T. Ersez, S. J. Kennedy and T. R. Finlayson, Polarised neutron scattering study of magnetic correlations and spin dynamics in $La_{0.875}Sr_{0.125}MnO_{3+d}$, Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s725-s727 (2002).
14. J. Garvey, Reactor Casts Light on Nanostructures, Australasian Science, 23, 19-23 (2002).
15. E.P. Gilbert, Modulated Structure Formation in Demixing Paraffin Blends, Applied Physics A Materials Science & Processing, 74 [Suppl1], s339-s341 (2002).
16. J. Goossens and L. D. Cussen, Optimising Neutron Polarizers - Measuring the Flipping Ratio and Related Quantities, Nuclear Instruments and Methods A 481, 475-492 (2002).
17. D. J. Goossens and L. D. Cussen, Optimising Neutron Polarizers - Measuring a Single Cross-Section, Nuclear Instruments and Methods A 490, 316-333 (2002).
18. E. M. Gray, L. D. Cussen, A. P. Murani and S. J. Kennedy, Magnetic scattering in irradiated $MnCu_4$ Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s935-s936 (2002).
19. T. W. Hambley, A. Katsifis, R. B. Knott, F. Mattner and B. Dikic, The Structures of Imidazenil and Iodoimidazenil, Aust. J. Chem. 55, 737-739 (2002).
20. P. Jackson, K. J. Fisher, I. G. Dance, G. E. Gadd and G. D. Willett, The structure of gas phase tin oxide ions generated by laser ablation: A combined Fourier transform mass spectrometry and density functional theory study, J. Cluster Sci., 13, 165-187 (2002).
21. M. James, The Structure and Magnetic Properties of the Two-Dimensional Di-Pyrazine Bridged Polymers $M(pz)_2Br_2$ (M = Fe(II), Co(II), Ni(II)), Australian Journal of Chemistry 55, 219-223 (2002).
22. M. James and J. Horvat, The Crystal Structure and Magnetic Properties of the 1-Dimensional Dihalide-Bridged Polymers Dichlorobis(thiazole)cobalt(II) and Dibromobis(thiazole)-cobalt(II), J. Physics and Chemistry of Solids 63, 657-663 (2002).
23. M. James and J. N. Watson, The Synthesis and Crystal Structure of Doped Uranium Brannerite Phases $U_{1-x}M_xTi_2O_6$ (M = Ca^{2+}, La^{3+} and Gd^{3+}), Journal of Solid State Chemistry 165, 261-265 (2002).
24. E. Kartini, S. J. Kennedy, T. Sakuma, K. Itoh, T. Fukunaga, M. F. Collins, T. Kamiyama, S. Suminta, A. Sugiharto, E. Musyafaah , P. Bawono, Structural, Thermal and Electrical Properties of AgI-Ag_2S-$AgPO_3$ Superionic Glasses Journal of Non-Crystalline Solids, 312-314, 628-632 (2002).
25. E. Kartini, S. Suminta, S. J. Kennedy, K. Itoh, T. Fukunaga and T. Kamiyama, Characterisation of the intermediate range order in new superionic conducting Ag_2S-AgI-$AgPO_3$ glasses by neutron diffraction, Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s1236-s1238 (2002).
26. B. J. Kennedy, B. A. Hunter and J. R. Hester, Synchrotron X-ray Diffraction Re-examination of the Sequence of High-Temperature Phases in $SrRuO_3$, Phys. Rev. B 65, 224101- 224104 (2002).
27. S. J. Kennedy, T. Kamiyama, K. Oikawa, S. J. Campbell and M. Hofmann, Magnetic phases in $La_{1-x}Mn_xMn_2Si_2$ High Resolution Diffraction, Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s880-s882 (2002).
28. S. J. Kennedy, B. A. Hunter, F. Mezei and L. Rosta, Design of neutron guide systems at the Australian Replacement research reactor, Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s40-s42 (2002).
29. W. Kockelmann, M. Hofmann, O. Moze, S. J. Kennedy and K. H. J. Buschow, Crystal structure and magnetic ordering of $RNi_{10}Si_2$ compounds, Eur. Phys. J. B., 30, 25-32 (2002)
30. J. Lal, E. P. Gilbert and L. Auvray, Confinement of Neutral and Charged Polymer Chains in Nanoporous Glass, Physica A 304 244-248 (2002).
31. V. Luca, J. Hanna, M. E. Smith, M. James, D. R. G. Mitchell and J. R. Bartlett, Nb-substitution and Cs^+ ion-exchange in Titanosilicate Sitinakite, Microporous and Mesoporous Materials 55, 1-13 (2002).
32. R. Macquart, B. J. Kennedy, B. A. Hunter and C. J. Howard, Structural Phase Transitions in the Ferroelectric Oxide $SrBi_2Ta_2O_9$, Integrated Ferroelectrics 44, 101-102 (2002).
33. R. Macquart, B. J. Kennedy, B. A. Hunter, C. J. Howard and Y. Shimakawa, High-Temperature Studies of $PbBi_2M_2O_9$, M=Nb and Ta, J. Phys.: Condens. Matter 14, 7955-7962 (2002).

34. S. M. Moussa, R. R. Fenton, B. A. Hunter and B. J. Kennedy, Polymorphism and Phase Transitions in bis(glycinato) copper(II). A Powder Diffraction Study, Australian J. Chemistry 55, 331-341 (2002).

35. O. Moze, J. M. Cadogan, S. J. Kennedy and K. H. J. Buschow, Magnetic Order in R_2Ni_{17} Intermetallics: a Neutron Diffraction Investigation, Physica B 319, 35-44 (2002).

36. M. Mulders, J. C. P. Klasse, D. J. Goossens, J. Chadwick and T. J. Hicks, High-Field Magnetization in the Diluted Quasi-two-dimensional Heisenberg Antiferromagnet $Mn_{1-x}Zn_xPS_3$, J. Phys.: Condens. Matter 14, 8697-8705 (2002).

37. Nakotte, R. A. Robinson, T. M. Kelley, S. Chang, T. Swan-Wood and E. Brűck, Inelastic Neutron Scattering Studies on UNiGe, Physica B 312-313, 875-876 (2002).

38. H. O'Connor, D. Y. Li and B. A. Hunter, The Importance of the Specimen Displacement Correction in Rietveld Pattern Fitting with Symmetric Reflection-Optics Diffraction Data, Advances in X-ray Analysis 44, 96-102 (2002).

39. V. K. Peterson, A. Ray, B. A. Hunter and L. P. Aldridge, Rietveld Refinement of Neutron, Synchrotron and Combined Powder Diffraction of Cement Clinker, Applied Physics A 74, [Suppl1], s1409-s1411 (2002).

40. M. P. Pitt, E. M. Gray and B. A. Hunter, Evolution of Microstructure in the $LaNi_{5-D}$ System during the Early Absorption-Desorption Cycles, J. Alloys Compounds 330-332, 241-245 (2002).

41. S. Pratapa, B. O'Connor and B. A. Hunter, A Comparative Study of Single-Line and Rietveld Strain-Size Evaluation Procedures using MgO Ceramics, J. Appl. Cryst. 35, 155-162 (2002).

42. K. Prodjosantoso, B. J. Kennedy and B. A. Hunter, Phase Separation Induced by Hydration of the Mixed Ca/Sr Aluminates $Ca_{3-x}Sr_xAl_2O_6$: A Crystallographic Study, Cement and Concrete Research 32, 647-655 (2002).

43. R. A. Robinson and S. J. Kennedy, Neutron Scattering at Australia's Replacement Research Reactor, Physica B, 311 44-49 (2002).

44. K. C. Rule, S. J. Kennedy, D. J. Goossens, A. M. Mulders and T. J. Hicks, Contrasting antiferromagnetic order between $FePS_3$ and $MnPS_3$, Applied Physics Letters A, Material Science & Processing, 74 [Suppl1], s811-s813 (2002).

45. J.C. Schulz & G.G. Warr, Adsorbed Layer Structure of Cationic and Anionic Surfactants on Mineral Oxide Surfaces, Langmuir 18, 3191-3197, (2002).

46. K. S. Wallwork, A. Pring, M. R. Taylor and B. A. Hunter, The structure of priceite, a basic hydrated calcium borate, by ab initio powder-diffraction methods, Canadian Mineralogist 40, 1199-1206 (2002).

47. W.H. Wang, E. Wu, R.J. Wang, S.J. Kennedy and A.J. Studer, Phase transformation in a $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$ bulk amorphous alloy upon crystallization. Physical Review B. 66, 104205, (2002).

48. X. L. Wang, M. James, J. Horvat, F. Gao, H. K. Liu and S. X. Dou, Structure and Spin Glass Behaviour in Non-Metallic Yb_2CoMnO_6 Perovskite Manganite, Journal of Magnetism and Magnetic Materials 246, 86-92 (2002).

49. X. L. Wang, M. James, J. Horvat, F. Gao, E. Sotirova, A. H. Li, H. K. Liu and S. X. Dou, Spin Glass Behaviour in Ferromagnetic La_2CoMnO_6 Perovskite, Superconductor Science and Technology 15, 427-430 (2002).

2003

1. R. A. Alderden, M. D. Hall, S. Amjadi, T. W. Hambley, P. Beale, M. Zhang, B. Lai, A. P. J. Stampfl, Increasing the cellular accumulation of platinum(IV) complexes, Journal of Inorganic Biochemistry, 96, 89 (2003).

2. N. Aleksandrovskii, A. Bakai, A. V. Dolbin, V. B. Esel'son, G. E. Gadd, V. G. Gavrilko, V. G. Manzhelii, S. Moricca, B. Sundqvist and B. G. Udovidchenko, Low-Temperature Thermal Expansion of Pure and Inert Gas-Doped Fullerite C_{60}, Low Temperature Physics 29, 324-332 (2003).

3. F. J. Brink, L. Noren, D. J. Goossens, R. L. Withers, Y. Liu and C. N. Xu, A Combined Diffraction (XRD, Electron and Neutron) and Dielectric Study of $Na_3MoO_3F_3$, J. Solid State Chemistry 174, 450-458 (2003).

4. A. N. Buckley, A. J. Hartmann, R. N. Lamb, A. P. J. Stampfl, J. W. Freeland and I. Coulthard, Threshold Al KLL Auger spectra of oxidised aluminium foils, Surface and Interface Anlaysis 35, 922-931 (2003).

5. R. P. Burford, M. G. Markotsis and R. B. Knott, Small-Angle Neutron Scattering and Transmission Electron Microscopy Studies of Interpenetrating Polymer Networks from Thermoplastic Elastomers, Nucl. Instrum. Meth. B 208, 58-65 (2003).

6. C. Burger, S. Ran, D. F. Fang, D. Cookson, K. Yabuki, Y. Teramoto, P. M. Cuniff, P. J. Viccaro, B. S. Hsiao and B. Chu, Time-Resolved Structural Studies in Fiber Processing, Macromol. Symp. 195, 297-302 (2003).

7. S. L. Cram, G. M. Spinks, G. G. Wallace and H. R. Brown, Electrochemical Polymerisation of Acrylics on Stainless Steel Cathodes, Journal of Applied Polymer Science 87, 765-773, (2003).

8. L. D. Cussen, Scan profiles for neutron spectrometers 1: Gaussian profile elements by acceptance diagram methods, Journal of Applied Crystallography 36, 1204-1213 (2003)

9. L. D. Cussen, Scan profiles for neutron spectrometers 2: Rectangular profile elements by acceptance diagram methods, Journal of Applied Crystallography 36, 1214-1224 (2003)

10. L. D. Cussen and A. R. Wildes, Scan profiles for neutron spectrometers 3: Rectangular profile elements by numerical methods, Journal of Applied Crystallography 36, 1225-1229 (2003)

11. H. De Bruyn, R. G. Gilbert, J. W. White and J. C. Schulz, SANS Study of Electrosterically Stabilized Polystyrene Latex, Polymer 44, 4411-4420 (2003).

12. C. T. Dillon, B. J. Kennedy, P. A. Lay, B. Lai, Z. Cai, A. P. J. Stampfl, P. Ilinski, D. G. Legnini, J. Maser, W. Rodrigues, G. Shea-McCarthy and M. Cholewa, Implementation of X-Ray Microscopy and Micro-XANES Analysis for Investigations of the Cellular Uptake and Cellular Metabolism of Transition Metals, Journal de Physique IV 104, 293-296 (2003).

13. T. Ersez, S. J. Kennedy, T. J. Hicks, Y. Fei, Th. Krist and P.A. Miles, New Features of the Long-Wavelength Polarisation Analysis Spectrometer - LONGPOL, Physica B 335, 183-187 (2003).

14. D. E. Fleming, A. van Riessen, M. C. Chauvet, P. K. Grover, B. A. Hunter, R. L. Ryall and W. van Bronswijk, Intracrystalline proteins and urolithiasis: a synchrotron x-ray diffraction study of calcium oxalate monohydrate, J. Bone and Min. Res. 18(7), 1282-1291 (2003).

15. C. J. Garvey, E. P. Gilbert, J. C. Schulz and R. B. Knott, Small-Angle Neutron Scattering Research at ANSTO, Neutron News 14(4), 27-31 (2003).

16. M. D. Hall, C. T. Dillon, M. Zhang, P. Beale, Z. Cai, B. Lai, A. P. J. Stampfl, T. W. Hambley, The cellular distribution and oxidation state of platinum(II) and platinum(IV) antitumour complexes in cancer cells, , J. Biol. Inorg. Chem., 8, 726-732, (2003).

17. M. D. Hall, T. W. Hambley, P. Beale, M. Zhang, C. T. Dillon, G. J. Foran, A. P. J. Stampfl and B. Lai, Does platinum(IV) survive in tumour cells?, Journal of Inorganic Biochemistry, 96(1), 141 (2003).

18. D. E. Hibbs, J. R. Hanrahan, M. B. Hursthouse, D. W. Knight, J. Overgaard, P. Turner, R. O. Piltz and M. P. Waller, Experimental and theoretical charge distribution in (Z)-N-methyl-C-phenylnitrone, Organic & Biomolecular Chemistry 1, 1034-1040 (2003).

19. D. E. Hibbs, J. Overgaard and R. O. Piltz, X-N Charge Density Analysis of 1-(2-hydroxy-5-nitrophenyl) ethanone, Organic & Biomolecular Chemistry 1, 1191-1198 (2003).

20. B. A. Hunter and B. J. Kennedy, Powder Diffraction in Australia, Neutron News 14(4), 19-21 (2003).

21. P. Ilinski, B. Lai, Z. Cai, W. Yun, D. Legnini, T. Talarico, M. Cholewa, L. K. Webster, G. B. Deacon, S. Rainone, D. R. Phillips and A. P. J. Stampfl, The direct mapping of the uptake of platinum anticancer agents in individual human ovarian adenocarcinoma cells using a hard x-ray microprobe, Cancer Research, 63(8), 1776-1779 (2003).

22. M. James, M. L. Carter and J. N. Watson, The Synthesis, Crystal Chemistry and Structures of Y-Doped Brannerite ($U_{1-x}Y_xTi_2O_6$) and Thorutite ($Th_{1-x}Y_xTi_2O_{6-d}$) Phases, J. Solid State Chem., 174, 329-333 (2003).

23. B. J. Kennedy, Y. Kubota, B. A. Hunter, Ismunandar and K. Kata, Structural Phase Transitions in the Layered Bismuth Oxide $BaBi_4Ti_4O_{15}$, Solid State Communications, 126(12), 653-658 (2003).

24. O. Kirstein, The Residual-Stress Diffractometer at the Australian Replacement Research Reactor, J. Neutron Research 11, 283-287 (2003).

25. E. H. Kisi, R. O. Piltz, J. S. Forrester and C. Howard, The Giant Piezo-Electric Effect: E-field Induced Monoclinic Phase or Piezoelectric Distortion of the Rhombohedral Parent?, J. Phys. Condens. Matter 15, 3631-3640 (2003).

26. I. McNulty, D. Paterson, J. Arko, M. Erdmann, S. P. Frigo, K. Goetze, P. Ilinski, N. Krapf, T. Mooney, C. C. Retsch, A. J. P. Stampfl, S. Vogt, Y. Wang, and S. Xu, The 2-ID-B Intermediate-Energy Scanning X-ray Microscope at the APS, Journal de Physique IV, 104, 11-15 (2003).

27. G. Paglia, C.E. Buckley, A.L. Rohl, B.A. Hunter, R.D. Hart, J.V. Hanna and L.T. Byrne, Tetragonal Structure Model for Boehmite-Derived γ-Alumina, Physical Review B 68, 144110 (2003).

28. V. K. Peterson, A. Ray, and B. Hunter, Importance of minor phase inclusion in the Rietveld analysis of cement clinkers, In Proceedings of the 11th International Congress on the Chemistry of Cement (Durban 2003), Cement and Concrete Institute, Durban, 146-150 (2003).

29. J. W. Phair, J. C. Schulz, W. K. Bertram, L. P. Aldridge, and J. S. J. van Deventer, Investigation of the Microstructure of Alkali-Activated Cements by Neutron Scattering, Cement and Concrete Research, 33, 1811-1824 (2003).

30. P. A. Reynolds, D. J. McGillivray, E. P. Gilbert, S. A. Holt, M. J. Henderson and J. W. White, Neutron and X-ray reflectivity from polyisobutylene-based amphiphiles at the air-water interface. Langmuir 19, 752-761 (2003).

31. R. A. Robinson and S. J. Kennedy, The Australian Replacement Research Reactor and the Bragg Institute, Neutron News 14(4), 14-18 (2003).

32. J. L. Ruggles, E. P. Gilbert, S. A. Holt, P. A. Reynolds and J. W. White, Expanded mesoporous silicate films grown at the air-water interface by addition of hydrocarbons, Langmuir 19, 793-800 (2003).

33. K. C. Rule, T. Ersez, S. J. Kennedy, T. J. Hicks, Identification of Features in the Powder Pattern of the Antiferromagnet $FePS_3$ Using Polarisation Analysis with Energy Analysis, Physica B: Condensed Matter, 335, 6-10 (2003).

34. S. Saricilar, R. B. Knott, C. Barner-Kowollik, T. Davis and J. Heuts, Reversible Addition Fragmentation Chain Transfer Polymerization of 3-[tris(trimethylsilyloxy) silyl]propyl methacrylate, Polymer 44, 5169-5176 (2003).

35. J. C. Schulz and M. James, Neutron Reflectometry in Australia: Science and Capabilities, Neutron News 14(4), 22-26 (2003).

36. J. R. Sun , J. Gao, Y. Fei, R. W. Li, and B. G. Shen, Doping effects on the phase separation in perovskite $La_{0.67-x}Bi_xCa_{0.33}MnO_3$, Phys. Rev. B 67, 144414-1 (2003).

37. V. A. Tolhurst, D. Cookson and P. Turner, A Synchrotron Study of mu(3)-chloro-tri-mu-chloro-mu(3)-sulfido-hexakis(triphenylphospine) trirunthenium(II)-tetrahydrofuran-water (1/1.25/0.75), Acta Cryst. E 59, M218-M219 (2003).

38. E. R. Vance, J. V. Hanna, B. A. Hunter, B. D. Begg, D. S. Perera, H. Li, Z. M. Zhang, Substitution of Zr, Mg, Al, Fe, Mn, Co and Ni in zirconolite, $CaZrTi_2O_7$. Ceramic Transactions , 143 (Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries VIII), 313-320 (2003).

39. K. S. Wallwork, A. Pring, M. R. Taylor and B. A. Hunter, A model for the structure of the hydrated aluminum phosphate, kingite determined by ab-initio powder diffraction methods, American Mineralogist 88, 235-239 (2003).

40. T. R. Welberry, D. J. Goossens, D. R. Haeffner, P. L. Lee and J. Almer, High-Energy Diffuse Scattering on the 1-ID-C beamline at the Advanced Photon Source, J. Synchrotron Radiation, 10, 284-286 (2003)

41. T. R. Welberry, D. J. Goossens, W. I. F. David, M. J. Gutmann, M. J. Bull and A. P. Heerdegen, Diffuse Neutron Scattering in Benzil, $C_{14}D_{10}O_2$, using the Time-of-Flight Laue Technique, J. Appl. Cryst. 36, 1440-1447 (2003).

42. R. L. Withers, M. James and D. J. Goossens, Atomic Ordering in the Doped Rare Earth Cobaltates $Ln_{0.33}Sr_{0.67}CoO_{3-d}$ (Ln = Y^{3+}, Ho^{3+} and Dy^{3+}), Journal of Solid State Chemistry, 174, 198-208 (2003).

43. E. Wu, S. J. Campbell, W. A. Kaczmarek, M. Hofmann and S. J. Kennedy, Nanostructured $(Co_xFe_{1-x})_{3-y}O_4$ spinel - mechanochemical synthesis, Zeitschrift fuer Metallkunde, 94, 1127-1133 (2003).

44. K. Wurst, E. Schweda, D. J. M Bevan, J. Mohyla, K. S. Wallwork, M. Hofmann, Single-crystal structure determination of $Zr_{50}Sc_{12}O_{118}$, Solid State Sciences, 5(11-12), 1491-1497 (2003).

45. D. H. Yu and M. Donath, Probing electron confinement in ultra-thin metal films: from spin-polarised quantum-well states to surface resonances, Europhysics Letters, 63, 729 (2003).

46. D. H. Yu, M. Donath, J. Braun and G. Rangelov, Spin-polarized unoccupied quantum-well states in ultrathin Co films on Cu(100), Phys. Rev. B, 68, 155415 (2003).

2004

1. D. B. Akolekar, G. Foran, and S. K. Bhargava, X-ray absorption spectroscopic studies on gold nanoparticles in mesoporous and microporous materials, Journal of Synchrotron Radiation, 11, 284-290 (2004).

2. P. Bendeich, C. Curfs, O. Kirstein, G. Atkinson, R. Rogge, Residual Stress Measurements of Laser-Clad Stainless Steel Coupons, Proc. 1st Int. Conf. Apl. of Lasers and Optics, editors M. Brandt and E. Harvey, in Press (2004).

3. A. Bennett, P. J. Daivis, R. Shanks, and R. Knott, Concentration dependence of static and hydrodynamic screening lengths for three different polymers in a variety of solvents, Polymer, 45, 8531-8540 (2004).

4. A. J. Berry, H. S. O'Neill, and G. J. Foran, The in situ determination of redox states in silicate melts, Lithos, 73, S9-S9 (2004).

5. T. Böcking, M. James, H. G. L. Coster, T. C. Chilcott and K. D. Barrow, Structural Characterization of Organic Multilayers on Silicon (111) Formed by Immobilization of Molecular Films on Functionalized Si-C Linked Monolayers, Langmuir, 20, 9227-9235 (2004).

6. C. T. Chantler, C. Q. Tran, and D. J. Cookson, Precise measurement of the lattice spacing of LaB_6 standard powder by the x-ray extended range technique using synchrotron radiation, Phys. Rev. A. 69, 2101-2101 (2004).

7. A. Cheung, G. D. Azevedo, C. J. Glover, D. J. Llewellyn, R. G. Elliman, G. J. Foran, and M. C. Ridgway, Structural perturbations within Ge nanocrystals in silica, Applied Physics Letters, 84, 278-280 (2004).

8. D. C. Creagh, G. Thorogood, M. James and D. L. Hallam, Diffraction and fluorescence studies of bushranger armour, Radiation Physics and Chemistry, 71, 839-840 (2004).

9. M. Donath and D. H. Yu, Electron confinement in metallic quantum wells probed by spin-resolved inverse photoemission, in Proceedings of the International Symposium on Synchrotron Radiation Research for Spin and Electronic States in d and f Electron Systems, SRSES2003, Nov. 19-21, 2003, Higashi-Hiroshima, Japan.

10. M. Donath and D. H. Yu, Electron confinement in metallic quantum-wells probed by spin-resolved inverse photoemission, Physica B-Condensed Matter, 351, 319-323 (2004).

11. T. Ersez, J.C. Schulz and T.R. Finlayson, Neutron Scattering Studies Of $La_{1-x}Sr_xMnO_3$ Colossal Magnetoresistive Perovskites, Materials Forum, 27, 80-87 (2004).

12. B. Etschmann, A. Pring, A. Putnis, B. A. Grguric and A. Studer, A Kinetic Study of Pentlandite $(Ni,Fe)_9S_8$ from the Monosulfide Solid Solution (Fe,Ni)S: Anneal-quench Experiments, American Mineralogist 89, 39-50 (2004).

13. H. Fansuri, D. K. Zhang, D. French, M. Elcombe and A. J. Studer, An X-Ray and Neutron Diffraction Study of the Structure of a- $Bi_2Mo_3O_{12}$ as a Catalyst for Partial Oxidation of Propylene to Acrolein, in Proceedings of CHEMECA 2003, Adelaide (2004).

14. C. J. Garvey, R. B. Knott, E. Drabarek, and P. W. Kuchel, Shear-induced alignment of self-associated hemoglobin in human erythrocytes: small angle neutron scattering studies, European Biophysics Journal with Biophysics Letters, 33, 589-595 (2004).

15. C. J. Garvey, I. H. Parker, R. B. Knott, and G. P. Simon, Small angle scattering in the Porod region from hydrated paper sheets at varying humidities, Holzforschung 58, 473-479 (2004).

16. D. J. Goossens, R. A. Robinson and M. T. F. Telling, The Antiferromagnetic Structure of $BaPrO_3$, Physica B 352, 105-110 (2004).

17. D. J. Goossens, K. F. Wilson, M. James, A. J. Studer and X. L. Wang, Structural and magnetic properties of $Y_{0.33}Sr_{0.67}CoO_{2.79}$, Phys. Rev. B 69, 134411 (2004).

18. C. L. Harland, L. H. Lewis, Z. Chen, and B. M. Ma, Exchange coupling and recoil loop area in $Nd_2Fe_{14}B$ nanocrystalline alloys, J. Magn. Magn. Mater. 271, 53-62 (2004).

19. N. Hauser and A. Götz, Choosing an instrument control system for ANSTO, in Proceedings of NOBUGS 2004, 18 - 20 October 2004, Villigen, Switzerland.

20. T. J. Hicks, D. J. Goossens, S. J .Harker, A. M. Mulders and S. J. Kennedy, Spin-resolved neutron spectroscopy from the Heavy Fermion Compound $CeCu_6$, Physica B, 345, 86-88 (2004).

21. B. A. Hunter, B. J. Kennedy and T. Vogt, Magnetorestriction in a Simple Trivalent Manganese Perovskite, Phys. Rev. B, 69, 410-410 (2004).

22. M. James, D. Cassidy, D. J. Goossens and R. L. Withers, The Phase Diagram and Tetragonal Superstructures of the Rare Earth Cobaltate Phases $Ln_{1-x}Sr_xCoO_{3-d}$ (Ln = La^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}, Gd^{3+}, Y^{3+}, Ho^{3+}, Dy^{3+}, Er^{3+}, Tm^{3+} and Yb^{3+}), J. Solid State Chem., 177, 1886-1895 (2004).

23. M. James, D. Cassidy, K. F. Wilson, J. Horvat and R. L. Withers, Oxygen Vacancy Ordering and Magnetism in the Rare Earth Stabilised Perovskite Form of $SrCoO_{3-d}$, Solid State Sciences 6, 655-662 (2004).

24. E. Kartini, S. J. Kennedy, K. Itoh, T. Kamiyama, M. F. Collins, and S. Suminta, Anion effect on the structure of Ag_2S-$AgPO_3$ superionic glasses, Solid State Ionics, 167, 65-71 (2004).

25. E. N. Khatsko, A. Zheludev, L. M. Tranquada, W. T. Klooster, A. M. Knigavko and R. C. Srivastava, Neutron Scattering Study of the layered Ising Magnet $CsDy(MoO_4)_2$, Low. Temp. Phys. 30, 133-139 (2004).

26. O. Kirstein and M. Prager, The lattice and rotational dynamics of the methyl halides described by pair potentials based on Universal Force Fields, Journal of Chemical Physics, 120, 5199-5207 (2004).

27. W. T. Klooster, R. O. Piltz, T. Uda, B. V. Merinov and S. M. Haile, Structure Refinement and Chemical Analysis of $Cs_3Li(DSO_4)_4$, formerly '$Cs_{1.5}Li_{1.5}D(SO_4)_2$', J. Solid State Chemistry 177, 274-280, (2004).

28. P. Kluth, B. Johannessen, V. Giraud, A. Cheung, C. J. Glover, G. D. Azevedo, G. J. Foran, and M. C. Ridgway, Bond length contraction in Au nanocrystals formed by ion implantation into thin SiO_2, Applied Physics Letters, 85, 3561-3563 (2004).

29. T. Lam, A. Götz, F. Franceschini, N. Hauser, GumTree - A Java Based GUI Framework for Beamline Experiments, submitted to Journal of Neutron Research (2004).

30. Y. Lee, J. A. Hriljac, A. Studer, T. Vogt, Anisotropic compression of edingtonite and thomsonite to 6 GPa at room temperature, Phys Chem Minerals 31, 22-27 (2004).

31. A. Levina, R. Codd, G. J. Foran, T. W. Hambley, T. Maschmeyer, A. F. Masters, and P. A. Lay, X-ray absorption spectroscopic studies of chromium(V/IV/III)2-ethyl-2-hydroxybutanoato(2-/1-) complexes, Inorganic Chemistry, 43, 1046-1055 (2004).

32. A. Levina, G. J. Foran, D. I. Pattison, and P. A. Lay, X-ray absorption spectroscopic and electrochemical studies of tris(catecholato (2-))chromate (V/I V/III) complexes, Angewandte Chemie-International Edition, 43, 462-465 (2004).

33. L. Q. Li, B. J. Kennedy, Y. Kubota, K. Kato, and R. F. Garrett, Structures and phase transitions in $Sr_{1-x}Ba_xHfO_3$ perovskites, Journal of Materials Chemistry, 14, 263-273 (2004).

34. Y. Ma, E. H. Kisi, S. J. Kennedy and A. J. Studer, Tetragonal to Monoclinic Transformation in MG-PSZ under Uniaxial Compression studied by in-situ Neutron Diffraction J. Am. Ceram. Soc. 87, 465-472 (2004).

35. S. T. Mudie, K. M. Pavlov, M. J. Morgan, J. R. Hester, M. Tabuchi, and Y. Takeda, Collection of reciprocal space maps using imaging plates at the Australian National Beamline Facility at the Photon Factory, Journal of Synchrotron Radiation, 11, 406-413 (2004).

36. A. Nelson and T. Cosgrove, Dynamic light scattering studies of poly(ethylene oxide) adsorbed on laponite: Layer conformation and its effect on particle stability, Langmuir, 20, 10382-10388 (2004).

37. A. Nelson and T. Cosgrove, A Small-Angle Neutron Scattering Study of Adsorbed Poly(ethylene oxide) on Laponite, Langmuir, 20(6), 2298-2304 (2004).

38. M. T. Ng, T. C. Deivaraj, W. T. Klooster, G. J. McIntyre, and J. J. Vittal, Hydrogen-bonded polyrotaxane-like structure containing cyclic $(H_2O)_4$ in $[Zn(OAc)_2$(m-bpe)]$.2H_2O$: X-ray and neutron diffraction studies, Chemistry-a European Journal, 10, 5853-5859 (2004).

39. G. Paglia, C.E. Buckley, A.L. Rohl, R.D. Hart, K. Winter, A.J. Studer, B.A. Hunter, and J.V. Hanna, The Boehmite Derived g-Alumina System, 1: Structural Variation with Temperature." Chemistry of Materials, 16, 220-236 (2004).

40. B. Pejcic, R. De Marco, C. E. Buckley, C. F. Maitland, and R. Knott, A small angle neutron scattering and electrochemical impedance spectroscopy study of the nanostructure of the iron chalcogenide glass ion-selective electrode, Talanta 63, 149-157 (2004).

41. V. K. Peterson, A Rietveld refinement investigation of a Mg-stabilized triclinic tricalcium silicate using synchrotron X-ray powder diffraction data, Powder Diffraction, 19, 356-358 (2004).

42. V. K. Peterson, A. Ray and B. Hunter, Tricalcium Silicate T_1 and T_2 Polymorphic Investigations: Rietveld Refinement at Various Temperatures using Synchrotron Powder Diffraction Data, J. Am. Ceram. Soc., 87, 1625-1635 (2004).

43. J. W. Phair, J. C. Schulz, L. P. Aldridge and J. D. Smith, Small-angle Neutron Scattering (SANS) and Rheological Characterization of Aluminosilicate Hydrogels, Journal of the American Ceramic Society, 87, 129-137, (2004).

44. S. F. Ran, C. Burger, I. Sics, K. Yoon, D. F. Fang, K. S. Kim, C. Avila-Orta, J. Keum, B. Chu, B. S. Hsiao, D. Cookson, D. Shultz, M. Lee, J. Viccaro, and Y. Ohta, In situ synchrotron SAXS/WAXD studies during melt spinning of modified carbon nanofiber and isotactic polypropylene nanocomposite, Colloid Polym. Sci. 282, 802-809 (2004).

45. M. C. Ridgway, G. D. Azevedo, C. J. Glover, R. G. Elliman, D. J. Llewellyn, A. Cheung, B. Johannessen, D. A. Brett, and G. J. Foran, EXAFS characterisation of Ge nanocrystals in silica, Nucl. Instrum. Methods B. 218, 421-426 (2004).

46. P. S. Salamakha, O. L. Sologub, C. Rizzoli, J. R. Hester, J. Stepien-Damm, A. P. Goncalves, E. B. Lopes, and M. Almeida, Ternary RPt_4B (R = La, Ce, Pr, Nd) compounds; structural and physical characterisation, Intermetallics, 12, 1325-1334 (2004).

47. D. Sutton, T. Hanley, R. Knott, and D. Cookson, Small-angle X-ray scattering on the ChemMatCARS beamline at the Advanced Photon Source: a study of shear-induced crystallization in polypropylene, Journal of Synchrotron Radiation, 11, 505-507 (2004).

48. D. Sutton, J. L. Stanford and A J Ryan, Reaction-Induced Phase Separation in Polyoxyethylene / Polystyrene Blends: (1) Ternary Phase Diagram, J. Macromolecular Science: Physics B43, 219-232 (2004).

49. D. Sutton, J. L. Stanford and A. J. Ryan, Reaction-Induced Phase Separation in Polyoxyethylene / Polystyrene Blends: (2) Structure Development, J. Macromolecular Science: Physics B43, 233-251 (2004).

50. V. Ting, Y. Liu, L. Norén, R. L. Withers, D. J. Goossens, M. James and C. Ferraris, A structure, conductivity and dielectric properties investigation of $A_3CoNb_2O_9$ (A = Ca^{2+}, Sr^{2+}, Ba^{2+}) triple perovskites., J. Solid State Chem., 177, 4428-4442 (2004).

51. J. C. Tucek, O. Auciello, D. M. Gruen, R. Winarski, J. W. Freeland, N. Moldovan, D. C. Mancini and A. P. J. Stampfl, Studies of electron field emission processes from low work function Cu-Li edge emitters via photoelectron and field electron emission microscopy, Submitted to Applied Physics Letters, (2004).

52. J. C. Tucek, O. Auciello, D. M. Gruen, R. Winarski, J. W. Freeland, N. Moldovan, and D. C. Mancini and A.P.J. Stampfl, Electron field emission arrays characterized by synchrotron-based photoelectron emission microscopy, Submitted to Advances in Functional Materials, (2004).

53. C. T. T. Tuttle, S. A. Seabrook, L. E. Wise, A. Katsifis, R. B. Knott, and B. F. Yates, Molecular modelling and design of radiolabelled complexes for melanoma diagnosis, Australian Journal of Chemistry, 57, 87-96 (2004).

54. K. S. Wallwork, A. Pring, M. R. Taylor and B. A. Hunter, The hydrogen bonding network in deuterated kingite as revealed by a neutron-diffraction investigation of its deuterated analogue, $Al_3(PO_4)2F_3{*}7D_2O$, Canadian Mineralogist, 42(1), 135-141 (2004).

55. X. L. Wang, S. Soltanian, M. James, Q. W. Yao, M. J. Qin, J. Horvat, H. K. Liu and S. X. Dou, Significant enhancement of critical current density and flux pinning in MgB_2 with nano-SiC, Si, and C doping,, Physica C, 408-410, 63-67 (2004).

56. J. F. Williams and D. H. Yu, Electron exchange in dissociative excitation of molecular hydrogen using polarized electrons, Physical Review Letters, 9307, 3201-3201 (2004).

57. H. Zhang, M. Hofmann, S. J. Kennedy and S. J. Campbell, The magnetic structure of the rare-earth intermetallic compound $La_3Co_{29}Si_4B_{10}$, in Materials Research Society Symposium Proceedings, 804(Combinatorial and Artificial Intelligence Methods in Materials Science II), 39-44 (2004).

2005

1. M. Ain, L. P. Regnault, J. Lorenzo, G. Dhalenne, and A. Reveolevschi, $CuGeO_3$ and CuO by respectively elastic and inelastic polarized neutrons, Physica B-Condensed Matter, 356, 60-63 (2005).

2. D. B. Akolekar, S. K. Bhargava, G. Foran, and M. Takahashi, Studies on gold nanoparticles supported on iron, cobalt, manganese, and cerium oxide catalytic materials, Journal of Molecular Catalysis A-Chemical, 238, 78-87 (2005).

3. N. Aleksandrovskii, A. V. Dolbin, V. B. Esel'son, V. G. Gavrilko, V. G. Manzhelii, A. S. Bakai, D. Cassidy, G. E. Gadd, S. Moricca, and B. Sundqvist, On the polyamorphism of fullerite-based orientational glasses, Low Temperature Physics, 31, 429-444 (2005).

4. P. W. Barnes, M. Avdeev, J. D. Jorgensen, D. G. Hinks, H. Claus, and S. Short, Superconductivity and cobalt oxidation state in metastable $Na_xCoO_{2-d}{\bullet}yH_2O$ (x approximate to 1/3; y approximate to 4x), Physical Review B, 72(13), 4515 (2005).

5. A. J. Berry, J. Hermann, H. S. C. O'Neill, and G. J. Foran, Fingerprinting the water site in mantle olivine, Geology, 31, 869-872 (2005).

6. T. Bocking, K. A. Kilian, T. Hanley, S. Ilyas, K. Gaus, M. Gal, and J. J. Gooding, Formation of tetra(ethylene oxide) terminated Si-C linked monolayers and their derivatization with glycine: An example of a generic strategy for the immobilization of biomolecules on silicon, Langmuir, 21, 10522-10529 (2005).

7. H. G. Brokmeier, B. Weiss, S. B. Yi, W. Y. Yi, K. D. Liss, and T. Lippmann, Texture determination of thin Cu-wires by synchrotron radiation, Materials Science Forum, 495-497, 131-136 (2005).

8. C. Curfs, O. Kirstein, A. J. Studer, R. Blevins, D. G. Carr, and M. I. Ripley, Residual stress measurements in Australia: Present and future, Materials Science Forum, 490-491, 218-222 (2005).

9. B. Dabrowski, S. Kolesnik, O. Chmaissem, T. Maxwell, M. Avdeev, P. W. Barnes, and J. D. Jorgensen, Increase of ferromagnetic ordering temperature by the minority-band double-exchange interaction in $SrRu_{1-x}Cr_xO_3$, Physical Review B, 72(5), 4428 (2005).

10. M. D. de Jonge, C. Q. Tran, C. T. Chantler, Z. Barnea, B. B. Dhal, D. J. Cookson, W. K. Lee, and A. Mashayekhi, Measurement of the x-ray mass attenuation coefficient and determination of the imaginary component of the atomic form factor of molybdenum over the 13.5-41.5-keV energy range, Physical Review A, 71 (2005).

11. R. A. Evans, T. L. Hanley, M. A. Skidmore, T. P. Davis, G. K. Such, L. H. Yee, G. E. Ball, and D. A. Lewis, The generic enhancement of photochromic dye switching speeds in a rigid polymer matrix, Nature Materials, 4, 249-253 (2005).

12. Y. Fei, S. J. Kennedy, S. J. Campbell, and M. Hofmann, Neutron polarization analysis of nanostructured $ZnFe_2O_4$, Physica B-Condensed Matter, 356, 264-268 (2005).

13. B. Finnigan, K. Jack, K. Campbell, P. Halley, R. Truss, P. Casey, D. Cookson, S. King, and D. Martin, Segmented polyurethane nanocomposites: Impact of controlled particle size nanofillers on the morphological response to uniaxial deformation, Macromolecules, 38, 7386-7396 (2005).

14. L. S. Fomenko, S. V. Lubenets, V. D. Natsik, D. Cassidy, G. E. Gadd, S. Moricca, and B. Sundqvist, Low-temperature microhardness of Xe-intercalated fullerite C_{60}, Low Temperature Physics, 31, 454-458 (2005).

15. J. S. Forrester, E. H. Kisi, and A. J. Studer, Direct observation of ferroelastic domain switching in polycrystalline $BaTiO_3$ using *in situ* neutron diffraction, Journal of the European Ceramic Society 25, 447-454 (2005).

16. S. Forster, A. Timmann, M. Konrad, C. Schellbach, A. Meyer, S. S. Funari, P. Mulvaney, and R. Knott, Scattering curves of ordered mesoscopic materials, Journal of Physical Chemistry B 109, 1347-1360 (2005).

17. E. P. Gilbert, A. Nelson, D. Sutton, N. Terrill, C. Martin, J. Lal, and E. Lang, Phase separation in the organic solid state: The influence of quenching protocol in unstable n-alkane blends, Molecular Crystals and Liquid Crystals, 440, 93-105 (2005).

18. C. J. Garvey, I. H. Parker, and G. P. Simon, On the interpretation of X-ray diffraction powder patterns in terms of the nanostructure of cellulose I fibres, Macromolecular Chemistry and Physics, 206, 1568-1575 (2005).

19. E. A. Goodilin, E. A. Pomerantseva, V. V. Krivetsky, D. M. Itkis, J. Hester, and Y. D. Tretyakov, A simple method of growth and lithiation of $Ba_6Mn_{24}O_{48}$ whiskers, Journal of Materials Chemistry, 15, 1614-1620 (2005).

20. D. J. Goossens, K. F. Wilson and M. James, Structure and magnetism in $Ho_{1-x}Sr_xCoO_{3-d}$, Journal of Physics and Chemistry of Solids 66, 169-175 (2005).

21. D. J. Goossens, X. D. Wu, and M. Prior, Structural phase transition in d-benzil characterised by capacitance measurements and neutron powder diffraction, Solid State Communications, 136, 543-545 (2005).

22. L. D. Graham, V. Glattauer, M. G. Huson, J. M. Maxwell, R. B. Knott, J. W. White, P. R. Vaughan, Y. Peng, M. J. Tyler, J. A. Werkmeister, and J. A. Ramshaw, Characterization of a protein-based adhesive elastomer secreted by the Australian frog Notaden bennetti, Biomacromolecules, 6, 3300-3312 (2005).

23. G. He, S. Gajjeraman, D. Schultz, D. Cookson, C. L. Qin, W. T. Butler, J. J. Hao, and A. George, Spatially and temporally controlled biomineralization is facilitated by interaction between self-assembled dentin matrix protein 1 and calcium phosphate nuclei in solution, Biochemistry, 44(49), 16140-16148 (2005).

24. G. He, A. Ramachandran, T. Dahl, S. George, D. Schultz, D. Cookson, A. Veis, and A. George, Phosphorylation of phosphophoryn is crucial for its function as a mediator of biomineralization, Journal of Biological Chemistry, 280, 33109-33114 (2005).

25. M. Hoelzel, V. Rajevac, S. A. Danilkin, T. J. Udovic, H. Wipf, and H. Fuess, Lattice dynamics of high-pressure hydrogenated austenitic stainless steels, Journal of Physics-Condensed Matter, 17, 3537-3546 (2005).

26. T. Itakura, W. K. Bertram, and R. B. Knott, The nanoscale structural response of a natural kaolinitic clayey soil subjected to uniaxial compression, Applied Clay Science, 29, 1-14 (2005).

27. M. James, A. Nelson, J. C. Schulz, M. J. Jones, M. Tran, and P. Hathaway, A New Neutron Reflectometer at Australia's HIFAR Research Reactor, Nuclear Instrum. Meth. A 536, 165-175 (2005).

28. M. James, T. Tedesco, D. J. Cassidy, and R. L. Withers, Oxygen vacancy ordering in strontium doped rare earth cobaltate perovskites $Ln_{1-x}Sr_xCoO_{3-d}$ (Ln = La, Pr and Nd; x > 0.60), Materials Research Bulletin, 40, 990-1000 (2005).

29. M. James, K. S. Wallwork, R. L. Withers, D. J. Goossens, K. F. Wilson, J. Horvat, X. L. Wang and M. Colella, Structure and magnetism in the oxygen-deficient perovskites $Ce_{1-x}Sr_xCoO_{3-d}$ (x > 0.90), Materials Research Bulletin, 40, 1415-1431 (2005).

30. B. Johannessen, P. Kluth, C. J. Glover, G. D. Azevedo, D. J. Llewellyn, G. J. Foran, and M. C. Ridgway, Structural characterization of Cu nanocrystals formed in SiO_2 by high-energy ion-beam synthesis, Journal of Applied Physics, 98, 024307 (2005).

31. B. Johannessen, P. Kluth, C. J. Glover, G. J. Foran, and M. C. Ridgway, Irradiation induced defects in nanocrystalline Cu, Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 238, 276-280 (2005).

32. J. D. Jorgensen, M. Avdeev, D. G. Hinks, P. W. Barnes, and S. Short, Thermal expansion and compressibility in superconducting $Na_xCoO_2 \cdot 4xD_2O$ (x approximate to 1/3): Evidence for pressure-induced charge redistribution, Physical Review B, 72(22), 4515 (2005).

33. S. J. Kennedy, Polarized neutrons for Australian scientific research, Physica B-Condensed Matter, 356, 71-78 (2005).

34. O. Kirstein, M. Prager, R. M. Dimeo, and A. Desmedt, Rotational dynamics of methyl groups in m-xylene, Journal of Chemical Physics 122, 14502-14502 (2005).

35. S. M. Kluth, B. Johannessen, P. Kluth, C. J. Glover, G. J. Foran, and M. C. Ridgway, EXAFS comparison of crystalline/ continuous and amorphous/porous GaSb, Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 238, 264-267 (2005).

36. P. Kluth, B. Johannessen, C. J. Glover, G. J. Foran, and M. C. Ridgway, Disorder in Au and Cu nanocrystals formed by ion implantation into thin SiO_2, Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 238, 285-289 (2005).

37. T. Klimczuk, M. Avdeev, J. D. Jorgensen, and R. J. Cava, Effect of B-11 substitution on the superconductivity of $MgCNi_3$, Physical Review B, 71(18), 4512 (2005).

38. T. F. Koetzle, A. J. Schultz, R. Henning, A. Albinati, W. T. Klooster, B. E. Eichler, and P. P. Power, Neutron diffraction analysis of the first stable hydride derivative of a divalent group-14 metal, Comptes Rendus Chimie, 8, 1487-1490 (2005).

39. K. Lewis, C. Kealley, M.M. Elcombe, A. van Riessen, and B. Ben-Nissan, Neutron Diffraction Comparison of a Bone Derived Hydroxyapatite Bioceramic and Synthetic Hydroxyapatite. Journal of the Australasian Ceramic Society 41(2), 52-55, (2005)

40. Y. Lin, A. Boker, H. Skaff, D. Cookson, A. D. Dinsmore, T. Emrick, and T. P. Russell, Nanoparticle assembly at fluid interfaces: Structure and dynamics, Langmuir 21, 191-194 (2005).

41. P. Manurung, I. M. Low, B. H. O'Connor, and S. Kennedy, Effect of b-spodumene on the phase development in an alumina/ aluminium-titanate system, Materials Research Bulletin, 40, 2047-2055 (2005).

42. Nelson and T. Cosgrove, Small-angle neutron scattering study of adsorbed pluronic tri-block copolymers on laponite, Langmuir, 21, 9176-9182 (2005).

43. H. S. C. O'Neill, M. James, W. A. Dollase, and S. A. T. Redfern, Temperature dependence of the cation distribution in $CuAl_2O_4$ spinel, European Journal of Mineralogy, 17, 581-586 (2005).

44. J. B. Peng, G. T. Barnes, I. R. Gentle, and G. J. Foran, Structure and thermal stability of Langmuir-Blodgett films of barium arachidate, Colloids and Surfaces a-Physicochemical and Engineering Aspects 253, 65-75 (2005).

45. J. B. Peng, G. J. Foran, G. T. Barnes, and I. R. Gentle, The structure of ultrathin Langmuir-Blodgett films of cadmium behenate, Journal of Chemical Physics, 123, 705 (2005).

46. V. K. Peterson, Lattice parameter measurement using Le Bail versus structural (Rietveld) refinement: A caution for complex, low symmetry systems, Powder Diffraction, 20, 14-17 (2005).

47. M. Prager, H. Grimm, and O. Kirstein, Using phase-space transformation for an improved hybrid cold time-of-flight spectrometer, Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment, 554, 415-426 (2005).

48. A. I. Prokhvatilov, N. N. Galtsov, I. V. Legchenkova, M. A. Strzhemechny, D. Cassidy, G. E. Gadd, S. Moricca, B. Sundqvist, and N. A. Aksenova, Hysteretic phenomena in Xe-doped C_{60} from x-ray diffraction, Low Temperature Physics, 31, 445-448 (2005).

49. M. C. Ridgway, G. D. Azevedo, R. G. Elliman, C. J. Glover, D. J. Llewellyn, R. Miller, W. Wesch, G. J. Foran, J. Hansen, and A. Nylandsted-Larsen, Ion-irradiation-induced preferential amorphization of Ge nanocrystals in silica, Physical Review B, 71 (2005).

50. M. C. Ridgway, C. J. Glover, G. D. Azevedo, S. M. Kluth, K. M. Yu, and G. J. Foran, Structure in amorphous semiconductors: Extrinsic and intrinsic, Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 238, 294-301 (2005).

51. A. S. Risbud, L. P. Snedeker, M. M. Elcombe, A. K. Cheetham, and R. Seshadri, Wurtzite CoO, Chemistry of Materials, 17, 834-838 (2005).

52. L. E. Rodgers, P. J. Holden, R. B. Knott, K. S. Finnie, J. R. Bartlett, and L. J. R. Foster, Effect of sol-gel encapsulation on lipase structure and function: A small angle neutron scattering study, Journal of Sol-Gel Science and Technology, 33, 65-69 (2005).

53. J. T. Russell, Y. Lin, A. Boker, L. Su, P. Carl, H. Zettl, J. B. He, K. Sill, R. Tangirala, T. Emrick, K. Littrell, P. Thiyagarajan, D. Cookson, A. Fery, Q. Wang, and T. P. Russell, Self-assembly and cross-linking of bionanoparticles at liquid-liquid interfaces, Angewandte Chemie-International Edition, 44, 2420-2426 (2005).

54. C. G. Ryan, B. E. Etschmann, S. Vogt, J. Maser, C. L. Harland, E. van Achterbergh, and D. Legnini, Nuclear microprobe-synchrotron synergy: Towards integrated quantitative real-time elemental imaging using PIXE and SXRF, Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 231, 183-188 (2005).

55. A. P. J. Stampfl, C. H. Chen, S. C. Wang, M. L. Huang, and R. Klauser, A scanning photoemission microprobe study of the adsorption of cysteine on Pt{111}, Journal of Electron Spectroscopy and Related Phenomena, 144, 417-420 (2005).

56. D. Sutton, P. Wanrooij, T. Hanley, R. Burford, E. Heeley, and R. Knott, A morphological study of linear and branched poly(ethylene terephthalate) using transmission electron microscopy and small-angle X-ray scattering, Journal of Macromolecular Science-Physics, B44, 1153-1171 (2005).

57. C. Tenailleau, B. Etschmann, H. Wang, A. Pring, B. A. Grguric, and A. Studer, Thermal expansion of troilite and pyrrhotite determined by in situ cooling (873 to 373 K) neutron powder diffraction measurements, Mineralogical Magazine, 69, 205-216 (2005).

58. H. J. Tracy, J. L. Mullin, W. T. Klooster, J. A. Martin, J. Haug, S. Wallace, I. Rudloe, and K. Watts, Enhanced photoluminescence from group 14 metalloles in aggregated and solid solutions, Inorganic Chemistry, 44, 2003-2011 (2005).

59. K. S. Wallwork, B. J. Kennedy, Q. D. Zhou, Y. Lee, and T. Vogt, Pressure and temperature-dependent structural studies of Ba_2BiTaO_6, Journal of Solid State Chemistry, 178, 207-211 (2005).

60. H. Zhang, M Hofmann, S. J. Kennedy and S. J. Campbell, Magnetic structure of $Nd_3Co_{29}Si_4B_{10}$, J. Appl. Phys. 97, 10M502-3 (2005).

61. H. Zhang, S. J. Campbell, M. Hofmann, and S. J. Kennedy, A neutron scattering study of rare-earth intermetallic compound $La_3Co_{29}Si_4B_{10}$, Journal of Applied Physics, 98 (2005).

62. Q. D. Zhou, B. J. Kennedy, K. S. Wallwork, M. M. Elcombe, Y. Lee, and T. Vogt, Temperature and pressure dependent structural studies of the ordered double perovskites $Sr_2TbRu_{1-x}Ir_xO_6$, Journal of Solid State Chemistry, 178, 2282-2291 (2005).

63. Q. D. Zhou, B. J. Kennedy, C. J. Howard, M. M. Elcombe, and A. J. Studer, Structural phase transitions in $A_{2-x}Sr_xNiWO_6$ (A = Ca or Ba, 0 <= x <= 2) double perovskites, Chemistry of Materials, 17, 5357-5365 (2005).

2006

1. D. B. Akolekar, S. K. Bhargava, and G. Foran, EXAFS studies on gold nanoparticles over novel catalytic materials, Radiat. Phys. Chem., 75(11), 1948-1952 (2006).

2. K. J. Alvine, D. Pontoni, O. G. Shpyrko, P. S. Pershan, D. J. Cookson, K. Shin, T. P. Russell, M. Brunnbauer, F. Stellacci, and O. Gang, Solvent mediated assembly of nanoparticles confined in mesoporous alumina, Phys. Rev. B 73, 125412 (2006).

3. R. S. Armstrong, G. J. Foran, W. A. Hough, D. M. D'Alessandro, P. A. Lay, and M. J. Crossley, Spectroelectrochemical evidence for communication within a laterally-bridged dimanganese(III) bis-porphyrin, Dalton Trans., 40, 4805-4813 (2006).

4. M. Avdeev, J. D. Jorgensen, S. Short, G. A. Samara, E. L. Venturini, P. Yang, and B. Morosin, Pressure-induced ferroelectric to antiferroelectric phase transition in $Pb_{0.99}(Zr_{0.95}Ti_{0.05})_{0.08}Nb_{0.2}O_3$, Phys. Rev. B, 73(6), Art. No. 064105 (2006).

5. M. Avdeev and V. B. Nalbandyan, New Cubic Perovskite $Na(Cu_{2.5}Ti_{0.5})Ti_4O_{12}$ with Square Planar Coordination of Ti4+, Inorg. Chem. 45, 2217-2220 (2006).

6. P. Bendeich, N. Alam, M. Brandt, D. Carr, K. Short, R. Blevins, C. Curfs, O. Kirstein, G. Atkinson, T. Holden, and R. Rogge, Residual stress measurements in laser clad repaired low pressure turbine blades for the power industry, Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process., 437(1), 70-74 (2006).

7. A. J. Berry, H. S. Neill, D. R. Scott, G. J. Foran, and J. M. G. Shelley, The effect of composition on Cr^{2+}/Cr^{3+} in silicate melts, Am. Miner., 91(11-12), 1901-1908 (2006).

8. A. J. Berry, H. O'Neill, and G. J. Foran, Electron exchange between V and Cr in silicate glasses, Geochim. Cosmochim. Acta, 70(18), A48-A48 (2006).

9. S. K. Bhargava, D. B. Akolekar, and G. Foran, X-ray absorption spectroscopic copper containing studies on novel microporous catalytic systems, Radiat. Phys. Chem., 75(11), 1909-1912 (2006).

10. T. Böcking, E. L. S. Wong, M. James, J. A. Watson, C. L. Brown, T. C. Chilcott, K. D. Barrow, and H. G. L. Coster, Immobilization of dendrimers on Si-C linked carboxylic acid-terminated monolayers on silicon(111), Thin Solid Films, 515(4), 1857-1863 (2006).

11. M. I. Bondin, S. J. Borg, M. H. Cheah, G. Foran, and S. P. Best, Integration of EXAFS, spectroscopic, and DFT techniques for elucidation of the structure of reactive diiron compounds, Aust. J. Chem. 59, 263-272 (2006).

12. P. D. Bonnitcha, M. D. Hall, C. K. Underwood, G. J. Foran, M. Zhang, P. J. Beale, and T. W. Hambley, XANES investigation of the Co oxidation state in solution and in cancer cells treated with Co(III) complexes, J. of Inorg. Biochem. 100, 963-971 (2006).

13. J. Brugger, B. Etschmann, Y. S. Chu, C. Harland, S. Vogt, C. Ryan, and H. Jones, The oxidation state of europium in hydrothermal scheelite: In situ measurement by xanes spectroscopy, Can. Mineral., 44, 1079-1087 (2006).

14. A. Brule and O. Kirstein, Residual stress diffractometer KOWARI at the Australian research reactor OPAL: Status of the project, Physica B 385-386, 1040-1042 (2006).

15. R. P. Burford, M. G. Markotsis and R. B. Knott, Real-time SANS study of interpenetrating polymer network (IPN) formation, Physica B 385-386, 766-769 (2006).

16. S. Carretta, P. Santini, G. Amoretti, T. Guidi, J. Dyson, R. Caciuffo, J. A. Stride, and A. Caneschi, Inelastic-neutron-scattering study of excited spin multiplets and low-energy phonons in the Fe-8 nanomagnet: Implications for relaxation, Phys. Rev. B 73, (2006).

17. M. Carter, K. Wallwork, M. James and R. Withers, Ab initio structure determinations of high-performance radioactive waste forms, Physica B 385-386, 535-537 (2006).

18. E. N. Caspi, M. Dubman, H. Ettedgui, H. Shaked, M. Melamud, L. Keller, and M. Avdeev, Magnetic and crystallographic properties of $TbCo_4B$, Physica B 385-386, 339-342 (2006).

19. J. Connolly, W. Bertram, J. Barker, C. Buckley, T. Edwards, and R. Knott, Comparison of the structure on the nanoscale of natural oil-bearing and synthetic rock, Journal of Petroleum Science and Engineering, 53(3-4), 171-178 (2006).

20. D. Cookson, N. Kirby, R. Knott, M. Lee, and D. Schultz, Strategies for data collection and calibration with a pinhole-geometry SAXS instrument on a synchrotron beamline, J. Synchrot. Radiat., 13, 440-444 (2006).

21. W. D. Cook, F. Chen, S. K. Ooi, C. Moorhoff, and R. Knott, Effect of curing order on the curing kinetics and morphology of bisGMA/DGEBA interpenetrating polymer networks, Polymer International, 55, 1027-1039 (2006).

22. M. B. Cortie, K. E. McBean and M. M. Elcombe, Fracture mechanics of mollusc shells, Physica B 385-386, 545-547 (2006).

23. J. E. Daniels, T. R. Finlayson, A. J. Studer, and M. E. Hagen, Time resolved studies near the ferroelectric transition in triglycine sulphate during the application of high-voltage fields, Ferroelectrics 339, 1861-1868 (2006).

24. J. E. Daniels, M. M. Elcombe, T. R. Finlayson and E. R. Vance, Neutron diffraction study of polycrystalline $Ca_{1-x}Sr_xTiO_3$ mixed perovskite materials, Physica B 385-386, 88-90 (2006).

25. J. E. Daniels, T. R. Finlayson, A. J. Studer and M. E. Hagen, Time-resolved neutron diffraction studies of triglycine sulphate near the ferroelectric transition during the application of high-voltage electric fields, Physica B 385-386, 97-99 (2006).

26. V. Darahanau, A. Benci, A. Y. Nikulin, J. Etheridge, J. Hester, and P. Zaumseil, High spatial resolution mapping of partially strain-compensated SiGe:C films in the presence of postannealed defects, J. Appl. Phys. 99, (2006).

27. R. A. Dilanian, A. Y. Nikulin, A. V. Darahanau, J. Hester, and P. Zaumseil, Application of phase-retrieval x-ray diffractometry to carbon doped SiGe(C)/Si(C) superlattice structures. II. High resolution reconstruction using neural network root finder technique, J. Appl. Phys. 99, (2006).

28. Y. D. Dong, I. Larson, T. Hanley, and B. J. Boyd, Bulk and dispersed aqueous phase behavior of phytantriol: Effect of vitamin E acetate and F127 polymer on liquid crystal nanostructure, Langmuir, 22(23), 9512-9518 (2006).

29. D. B. Drazkowski, A. Lee, T. S. Haddad, and D. J. Cookson, Chemical substituent effects on morphological transitions in styrene-butadiene-styrene triblock copolymer grafted with polyhedral oligomeric silsesquioxanes, Macromolecules 39, 1854-1863 (2006).

30. N. K. Dutta, S. R. Thompson, N. Choudhury and R. B. Knott, Environment-induced self-assembly in phase separated block copolymer systems: A SANS investigation, Physica B 385-386, 773-775 (2006).

31. S. El-Khatib, A. Llobet, A. Purwanto, R. A. Robinson, S. H. Lee, J. W. Lynn, S. Chang, and H. Nakotte, Magnetic structures in UCuSn, J. Appl. Phys., 99, 704 (2006).

32. B. Finnigan, P. Halley, K. Jack, A. McDowell, R. Truss, P. Casey, R. Knott, and D. Martin, Effect of the average soft-segment length on the morphology and properties of segmented polyurethane nanocomposites, Journal of Applied Polymer Science, 102(1), 128-139 (2006).

33. L. J. R. Foster, R. B. Knott, V. Sanguanchaipaiwong and P. J. Holden, Polyhydroxyalkanoate-based natural?synthetic hybrid copolymer films: A small-angle neutron scattering study, Physica B 385-386, 770-772 (2006).

34. C. J. Garvey, R. B. Knott, M. Searson, and J. P. Conroy, USANS study of wood structure, Physica B, 385-386, 877-879 (2006).

35. M. J. Gidley, B. M. Flanagan, A. Shrestha, A. Lopez Rubio, E. Gilbert, A. Htoon, H. Chanvrier, S. Uthayakumaran, P. J. Lillford, X. K. Zhou, A. R. Bird and D. L. Topping, Digestibility of starches: effects of polymer conformation and food structure, Asia Pacific J. Clinical Nutrition 15, S44 (2006).

36. E. M. Gray, D. J. Cookson, and T. P. Blach, X-ray diffraction cell for studying solid-gas reactions under gas pressures to 100 bar, J. Appl. Crystallogr., 39, 850-855 (2006).

37. E. P. Gilbert, J. C. Schulz and T. J. Noakes, 'QUOKKA' the small-angle neutron scattering instrument at OPAL, Physica B 385-386, 1180-1182 (2006).

38. M. D. Hall, R. A. Alderden, M. Zhang, P. J. Beale, Z. H. Cai, B. Lai, A. P. J. Stampfl, and T. W. Hambley, The fate of platinum(II) and platinum(IV) anti-cancer agents in cancer cells and tumours, J. Struct. Biology 155, 38-44 (2006).

39. W. A. Hamilton, G. S. Smith, G. B. Taylor, B. M. Larkins, and L. Porcar, Current and future capabilities of the neutron reflectometer MIRROR at Oak Ridge National Laboratory's High Flux Isotope Reactor, Physica B, 385-386, 1007-1009 (2006).

40. T. L. Hanley, J. S. Forsythe, D. Sutton, G. Moad, R. P. Burford, and R. B. Knott, Crystallisation kinetics of novel branched poly(ethylene terephthalate): a small-angle X-ray scattering study, Polym. Int., 55(12), 1435-1443 (2006).

41. T. Hanley, D. Sutton, D. Cookson, E. Kosior, and R. Knott, Molecular morphology of petaloid bases of PET bottles: A small-angle X-ray scattering study, J. Appl. Polymer Science 99, 3328-3335 (2006).

42. J. Healy, G. H. Edward and R. B. Knott, Residual orientation in injection micro-molded samples, Physica B 385-386, 620-622 (2006).

43. J. R. Hester, A validating CIF parser: PyCIFRW, J. Appl. Cryst., 39, 621-625 (2006).

44. R. M. Hough, C. G. Ryan, R. R. Anand, B. E. Etschmann, C. L. Harland, and F. DeCarlo, A Synchrotron based study of lateritic, gold bearing, iron oxide nodules, Geochim. Cosmochim. Acta, 70(18), A266-A266 (2006).

45. J. Hunger, I. A. Beta, H. Bohlig, C. Ling, H. Jobic, and B. Hunger, Adsorption structures of water in NaX studied by DRIFT spectroscopy and neutron powder diffraction, J. Phys. Chem. B, 110, 342-353 (2006).

46. W. D. Hutchison, D. J. Goossens, K. Nishimura, K. Mori, Y. ISIKAwa, and A. Studer, Magnetic structure of $TbNiAl_4$, J. Magn. Magn. Mater. 301, 352-358 (2006).

47. M. James, L. Morales, K. S. Wallwork, M. Avdeev, R. L. Withers, D. J. Goossens, Structure and magnetism in rare earth strontium-doped cobaltates, Physica B 385-386, 199-201 (2006).

48. M. James, A. Nelson, A. Brule, and J. C. Schulz, PLATYPUS: a time-of-flight neutron reflectometer at Australia's new research reactor, J. Neutron Research, 14(2), 91-108 (2006).

49. M. James, A. Tedesco, D. Cassidy, M. Colella, and P. J. Smythe, The phase diagram and crystal chemistry of strontium-doped rare earth cobaltates: $Ln_{2-x}Sr_xCoO_{4+d}$ (Ln = La-Dy), J. Alloys Compounds, 419(1-2), 201-207 (2006).

50. B. Johannessen, P. Kluth, D. J. Cookson, G. J. Foran, and M. C. Ridgway, Size-dependent structural disorder in nanocrystalline Cu probed by synchrotron-based X-ray techniques, Nuclear Instrum. Meth. B 246, 45-49 (2006).

51. B. Johannessen, P. Kluth, C. J. Glover, G. J. Foran, and M. C. Ridgway, Diffusion limited Cu and Au nanocrystal formation in thin film SiO_2, Nuclear Instrum. Meth. B 242, 133-136 (2006).

52. B. Johannessen, P. Kluth, C. J. Glover, S. M. Kluth, G. J. Foran, D. J. Cookson, D. J. Llewellyn, and M. C. Ridgway, Structural stability of Cu nanocrystals in SiO_2 exposed to high-energy ion irradiation, Nuclear Instrum. Meth. B 250, 210-214 (2006).

53. D. John, A. Blom, S. Bailey, A. Nelson, J. Schulz, R. De Marco, The application of neutron reflectometry and atomic force microscopy in the study of corrosion inhibitor films, Physica B 385-386, 924-926 (2006).

54. J. L. Jones, M. Hoffman, J. E. Daniels, and A. J. Studer, Direct measurement of the domain switching contribution to the dynamic piezoelectric response in ferroelectric ceramics, Applied Physics Letters, 89(9) (2006).

55. J. L. Jones, M. Hoffman, J. E. Daniels, and A. J. Studer, Ferroelastic contribution to the piezoelectric response in lead zirconate titanate by in situ stroboscopic neutron diffraction, Physica B 385-386, 100-102 (2006).

56. C. Kealley, M. Elcombe, A. van Riessen, and B. Ben-Nissan, Neutron Chracterisation of Hydroxyapatite Bioceramics 18, Pts 1 and 2; Vol. 309-311 (Trans Tech Publications LTD, Zurich-Uetikon, 2006), p. 61-64.

57. C. Kealley, M. Elcombe, A. van Riessen and B. Ben-Nissan, Development of carbon nanotube-reinforced hydroxyapatite bioceramics, Physica B 385-386, 496-498 (2006).

58. C. Kealley, B. Ben-Nissan, A. van Riessen, and M. Elcombe, in Bioceramics 18, Pts 1 and 2; Vol. 309-311 (Trans Tech Publications LTD, Zurich-Uetikon, 2006), p. 597-600.

59. S. J. Kennedy, Construction of the neutron beam facility at Australia's OPAL research reactor, Physica B 385-386, 949-954 (2006).

60. O. Kirstein, M. Prager, H. Grimm, A. Buchsteiner and A. Wischnewski, Quasi-elastic neutron spectroscopy and rotational potentials of methyl halides, Physica B 385-386, 47-49 (2006).

61. P. Kluth, B. Hoy, B. Johannessen, S. G. Dunn, G. J. Foran, and M. C. Ridgway, Co-Au core-shell nanocrystals formed by sequential ion implantation into SiO_2, Appl. Phys. Lett., 89(15), Art. No. 153118(2006).

62. P. Kluth, B. Johannessen, D. J. Cookson, G. J. Foran, and M. C. Ridgway, SAXS and EXAFS studies of ion beam synthesized Au nanocrystals, Nuclear Instrum. Meth. B 246, 30-34 (2006).

63. P. Kluth, B. Johannessen, G. J. Foran, D. J. Cookson, S. M. Kluth, and M. C. Ridgway, Disorder and cluster formation during ion irradiation of Au nanoparticles in SiO_2, Phys. Rev. B, 74(1), Art. No. 014202 (2006).

64. P. Kluth, B. Johannessen, S. M. Kluth, G. J. Foran, D. J. Cookson, and M. C. Ridgway, Structure and morphology of ion irradiated Au nanocrystals in SiO_2, Nuclear Instrum. Meth. B, 250, 215-219 (2006).

65. R. B. Knott, M. Lin, H. J. M. Hanley, and D. Muir, Preliminary SANS studies of the structure of nickel powders on the nanoscale, Physica B 385-386, 908-910 (2006).

66. T. Lam, A. Götz, F. Franceschini, and N. Hauser, GumTree - a Java based GUI framework for beamline experiments, J. Neutron Research 14, 167-175 (2006).

67. T. Lam, N. Hauser, A. Götz, P. Hathaway, F. Franceschini, H. Rayner, GumTree– An integrated scientific experiment environment, Physica B 385-386, 1330-1332 (2006).

68. C. Lau, R. Bitton, H. Bianco-Peled, D. G. Schultz, D. J. Cookson, S. T. Grosser, and J. W. Schneider, Morphological characterization of self-assembled peptide nucleic acid amphiphiles, J. Phys. Chem. B 110, 9027-9033 (2006).

69. M. Law, T. Gnapel-Herold, V. Luzin, and G. Bowie, Neutron residual stress measurements in linepipe, Physica B, 385-386, 900-903 (2006).

70. M. Law, H. Prask, V. Luzin, and T. Gnaeupel-Herold, Residual stress measurements in coil, linepipe and girth welded pipe, Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process., 437(1), 60-63 (2006).

71. L. H. Lewis, C. L. Harland, R. W. McCallum, M. J. Kramer, and K. W. Dennis, Phase-separated alloys for bulk exchange-biased permanent magnets, J. Appl. Phys. 99(8) (2006).

72. Q. S. Lin, M. Greenblatt, E. N. Caspi, and M. Avdeev, Crystallographic and magnetic properties of $CaLaMnMoO_6$ double perovskite, J. Solid State Chem., 179, 2086-2092 (2006).

73. C. D. Ling, Solving δ-Bi_2O_3-related superstructures by combining neutron powder diffraction and ab initio calculations, Physica B 385-386, 193-195 (2006).

74. K.-D. Liss, B. Hunter, M. Hagen, T. Noakes and S. Kennedy, ECHIDNA–the new high-resolution powder diffractometer being built at OPAL, Physica B 385-386, 1010-1012 (2006).

75. K.-D. Liss, A. Bartels, H. Clemens, S. Bystrzanowski, A. Stark, T. Buslaps, F.-P. Schimansky, R. Gerling, C. Scheu, and A. Schreyer, Recrystallization and phase transitions in a γ-TiAl-based alloy as observed by ex situ and in situ high-energy X-ray diffraction, Acta Materialia, 54(14), 3721-3735 (2006).

76. W. Liu, B. Etschmann, J. Brugger, L. Spiccia, G. Foran, and B. McInnes, UV-Vis spectrophotometric and XAFS studies of ferric chloride complexes in hyper-saline LiCl solutions at 25-90 degrees C, Chemical Geology, 231(4), 326-349 (2006).

77. W. Liu, B. Etschmann, G. Foran, M. Shelley, and J. Brugger, A XANES study of Zn and Fe(II) chloride complexes in hypersaline brines, Geochim. Cosmochim. Acta, 70(18), A364-A364 (2006).

78. A. Lopez-Rubio, E. Gimenez, R. Gavara, and J. M. Lagaron, Gas barrier changes and structural alterations induced by retorting in a high barrier aliphatic polyketone terpolymer, J. Appl. Polymer Science, 101(5), 3348-3356 (2006).

79. V. Luca, J. N. Watson, M. Ruschena, and R. B. Knott, Anionic surfactant templated titanium oxide mesophase: Synthesis, characterization, and mechanism of formation, Chemistry of Materials, 18, 1156-1168 (2006).

80. M. D. Lumsden, J. L. Robertson, and M. Yethiraj, SPICE - Spectrometer and Instrument Control Environment, Physica B, 385-386, 1336-1339 (2006).

81. R. Magaraggia, S. Kennedy, T. Tedesco, E. Kartini, M. Collins and K. Itoh, Reverse Monte-Carlo Analysis of neutron diffraction from AgI-Ag_2S-$AgPO_3$ superionic conducting glasses, Physica B 385-386, 263-265 (2006).

82. R. J. McQueeney, M. Yethiraj, W. Montfrooij, J. S. Gardner, P. Metcalf, and J. M. Honig, Possible large spin-phonon coupling in magnetite, Physica B, 385, 75-78 (2006).

83. C. Milsmann, A. Levina, H. H. Harris, G. J. Foran, P. Turner, and P. A. Lay, Charge distribution in chromium and vanadium catecholato complexes: X-ray absorption spectroscopic and computational studies, Inorg. Chem. 45, 4743-4754 (2006).

84. R. A. Mole, J. A. Stride, A. S. Wills and P. T. Wood, Static and dynamic properties of $Mn_2(OH)_2(C_4O_4)$, Physica B 385-386, 435-437 (2006).

85. L. Morales, A. Caneiro and M. James, Neutron powder diffraction study of nuclear and magnetic structures of $LaMn_{1-x}Cr_xO_{3.00}$ (x = 0.05 and 0.15), Physica B 385-386, 415-417 (2006).

86. A. M. Mulders, U. Staub, V. Scagnoli, S. W. Lovesey, E. Balcar, T. Nakamura, A. Kikkawa, G. van der Laan, and J. M. Tonnerre, High-order Dy multipole motifs observed in DyB_2C_2 with resonant soft x-ray Bragg diffraction, J. Phys.-Condes. Matter, 18(49), 11195-11202 (2006).

87. A. M. Mulders, U. Staub, V. Scagnoli, T. Nakamura, A. Kikkawa, and J. M. Tonnerre, Orbital order in DyB_2C_2 studied with resonant soft X-ray scattering, Physica B 378-80, 367-368 (2006).

88. V. B. Nalbandyan, M. Avdeev, and A. A. Pospelov, Ion exchange reactions of $NaSbO_3$ and morphotropic series $MSbO_3$, Solid State Sci., 8(12), 1430-1437 (2006).

89. A. Nelson, Co-refinement of multiple-contrast neutron/X-ray reflectivity data using MOTOFIT, J. Appl. Cryst. 39, 273-276 (2006).

90. A. Nelson, B. W. Muir, J. Oldham, C. Fong, K. M. McLean, P. G. Hartley, S. K. Oiseth, and M. James, X-ray and neutron reflectometry study of glow-discharge plasma polymer films, Langmuir, 22, 453-458 (2006).

91. B. O'Neill, C. Tenailleau, Y. Nogthai, A. Studer, J. Brugger, and A. Pring, A flow-through hydrothermal cell for in situ neutron diffraction studies of phase transformations, Physica B, 385-386, 942-945 (2006).

92. H. S. C. O'Neill, A. J. Berry, C. C. McCammon, K. D. Jayasuriya, S. J. Campbell, and G. Foran, An experimental determination of the effect of pressure on the Fe^{3+}/Sigma Fe ratio of an anhydrous silicate melt to 3.0 GPa, American Mineralogist, 91, 404-412 (2006).

93. S. Park, Y. Lee, M. Elcombe, and T. Vogt, Synthesis and structure of the bilayer hydrate $Na_{0.3}NiO_2 \cdot 1.3D_2O$, Inorg. Chem., 45, 3490-3492 (2006).

94. V. K. Peterson, Y. Liu, C. M. Brown, and C. J. Kepert, Neutron powder diffraction study of D-2 sorption in Cu-3(1,3,5-benzenetricarboxylate)(2), J. Am. Chem. Soc., 128(49), 15578-15579 (2006).

95. V. K. Peterson, A. S. Ray, and B. A. Hunter, A comparative study of Rietveld phase analysis of cement clinker using neutron, laboratory X-ray, and synchrotron data, Powder Diffraction, 21, 12-18 (2006).

96. R. O. Piltz, Domain structure of 001-poled PZN-4.5%PT using neutron diffraction, Ferroelectrics, 339, 1733-1737 (2006).

97. R. O. Piltz, Neutron diffraction study of domain structures in poled and unpoled PZN 4.5%PT, Physica B 385-386, 169-172 (2006).

98. M. Prager, H. Grimm, and O. Kirstein, A space and energy focusing hybrid cold time-of-flight spectrometer based on a moving monochromator crystal, Physica B 385-386, 1098-1100 (2006).

99. S. Ramachandran, J. Trewhella, Y. Tseng, and Y. B. Yu, Coassembling peptide-based biomaterials: Effects of pairing equal and unequal chain length oligopeptides, Chem. Mat., 18(26), 6157-6162 (2006).

100. H. Rayner, P. Hathaway, N. Hauser, Y. Fei, F. Franceschini and T. Lam, GumTree: Data reduction, Physica B 385-386, 1333-1335 (2006).

101. M. C. Ridgway, G. D. Azevedo, R. G. Elliman, W. Wesch, C. J. Glover, R. Miller, D. J. Llewellyn, G. J. Foran, J. L. Hansen, and A. N. Larsen, Preferential amorphisation of Ge nanocrystals in a silica matrix, Nuclear Instrum. Meth. B, 242, 121-124 (2006).

102. M. C. Ridgway, S. E. Everett, C. J. Glover, S. M. Kluth, P. Kluth, B. Johannessen, Z. S. Hussain, D. J. Llewellyn, G. J. Foran, and G. D. Azevedo, Atomic-scale structure of irradiated GaN compared to amorphised GaP and GaAs, Nuclear Instrum. Meth. B 250, 287-290 (2006).

103. M. I. Ripley and O. Kirstein, Residual stresses in a cast iron automotive brake disc rotor, Physica B, 385-386, 604-606 (2006).

104. L. E. Rodgers, R. B. Knott, P. J. Holden, K. J. Pike, J. V. Hanna, L. J. R. Foster and J. R. Bartlett, Structural evolution and stability of sol-gel biocatalysts, Physica B 385-386, 508-510 (2006).

105. R. A. Robinson, D. J. Goossens, M. S. Torikachvili, K. Kakurai and H. Okumura, A Quantum Multi-Critical Point in $CeCu_{6-x}Au_x$, Physica B 385-386, 38-40 (2006).

106. J. L. Ruggles, G. J. Foran, H. Tanida, H. Nagatani, Y. Jimura, I. Watanabe, and I. R. Gentle, Interfacial behavior of tetrapyridylporphyrin monolayer arrays, Langmuir, 22, 681-686 (2006).

107. J. Ruiz-Hervias, V. Luzin, H. Prask, T. Gnaeupel-Herold, and M. Elices, Effect of thermo-mechanical treatments on residual stresses measured by neutron diffraction in cold-drawn steel rods, Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process., 435, 725-735 (2006).

108. P. J. Saines, M. M. Elcombe, and B. J. Kennedy, Lanthanide distribution in some doped alkaline earth aluminates and gallates, J. Solid State Chem., 179, 613-622 (2006).

109. P. J. Saines, M. M. Elcombe and B. J. Kennedy, Structural studies of oxygen deficient lanthanide containing double perovskites, Physica B 385-386, 187-189 (2006).

110. V. Scagnoli, U. Staub, A. M. Mulders, G. I. Meijer, G. Hammerl, and J. M. Tonnerre, Magnetic and orbital ordering in $NdNiO_3$, Physica B, 378-80, 541-542 (2006).

111. O. A. Smirnova, M. Avdeev, V. B. Nalbandyan, V. V. Kharton, and F. M. B. Marques, First observation of the reversible O3 <-> P2 phase transition - Crystal structure of the quenched high-temperature phase $Na_{0.74}M_{0.58}Sb_{0.42}O_2$, Materials Research Bulletin, 41, 1056-1062 (2006).

112. O. A. Smirnova, V. B. Nalbandyan, A. A. Petrenko, and M. Avdeev, Subsolidus phase relations in Na_2O-CuO-Sb_2O_n system and crystal structure of new sodium copper antimonate $Na_3Cu_2SbO_6$, J. Solid State Chem. 179, 1293-1293 (2006).

113. U. Staub, V. Scagnoli, A. M. Mulders, M. Janousch, Z. Honda, and J. M. Tonnerre, Charge/orbital ordering vs. Jahn-Teller distortion in $La_{0.5}Sr_{1.5}MnO_4$, Europhys. Lett., 76(5), 926-932 (2006).

114. J. A. Stride, U. A. Jayasooriya, J. M. Zanotti, and R. Kahn, Molecular dynamics of the self-organising strong hydrogen bonded 3,5-dimethylpyrazole, New Journal of Chemistry, 30(3), 425-429 (2006).

115. J. A. Stride, M. Kurmoo, and Z. Wang, Investigations of guest-modulated ordering temperatures in open-framework 3D porous magnets, Physica B, 385-386, 465-467 (2006).

116. J. C. Stroud, Y. Q. Wu, D. L. Bates, A. D. Han, K. Nowick, S. Paabo, H. Tong, and L. Chen, Structure of the forkhead domain of FOXP2 bound to DNA, Structure, 14, 159-166 (2006).

117. J. Studer, M. E. Hagen and T. J. Noakes, WOMBAT: The high-intensity powder diffractometer at the OPAL reactor, Physica B 385-386, 1013-1015 (2006).

118. D.Tawfik, O. Kirstein, P. J. Mutton and W. K. Chiu, Verification of residual stresses in flash-butt-weld rails using neutron diffraction, Physica B 385-386, 894-896 (2006).

119. N. Tezuka, I.-T. Low, I. J. Davies, M. Prior and A. Studer, In-situ neutron diffraction investigation on the phase transformation sequence of kaolinite and halloysite to mullite, Physica B 385-386, 555-557 (2006).

120. V. Ting, Y. Liu, R. L. Withers, L. Noren, M. James, and J. D. F. Gerald, A structure and phase analysis investigation of the 1:1 ordered A_2InNbO_6 perovskites (A = Ca^{2+}, Sr^{2+}, Ba^{2+}) , J. Solid State Chem. 179, 551-562 (2006).

121. J. Trewhella, Protein kinase A targeting and activation as seen by small-angle solution scattering, European Journal of Cell Biology, 85(7), 655-662 (2006).

122. J. Trewhella, Structural themes and variations in protein kinase A as seen by small-angle scattering and neutron contrast variation, European Biophysics Journal with Biophysics Letters, 35(7), 585-589 (2006).

123. J. Trewhella, Neutrons reveal how nature uses structural themes and variation in biological regulation, Physica B 385-386, 825-830 (2006).

124. D. Vigil, D. K. Blumenthal, S. S. Taylor, and J. Trewhella, Solution scattering reveals large differences in the global structures of type II protein kinase a isoforms, J. Molec. Biology, 357(3), 880-889 (2006).

125. M. P. Waller, S. T. Howard, J. A. Platts, R. O. Piltz, D. J. Willock, and D. E. Hibbs, Novel properties from experimental charge densities: An application to the zwitterionic neurotransmitter taurine, Chem.-Eur. J., 12(29), 7603-7614 (2006).

126. K. S. Wallwork, M. James, and M. L. Carter, The crystal chemistry, structure and properties of a synthetic carnotite-type compound, $Ba_2(UO_2)_2Ti_2O_8$, Canadian Mineralogist, 44, 433-442 (2006).

127. J. L. Wang, S. J. Campbell, J. M. Cadogan, O. Tegus, A. J. Studer, and M. Hofmann, Magnetic properties of $PrMn_{2-x}Fe_xGe_2$ ^{57}Fe Mossbauer spectroscopy, J. Phys.: Condens. Matter 18, 189-204 (2006).

128. J. L. Wang, A. J. Studer, S. J. Campbell, M. Hofmann, and J. M. Cadogan, Magnetic properties of $PrMn_{1.2}Fe_{0.8}Ge_2$, Physica B 385-386, 326-329 (2006).

129. A. E. Whitten and M. A. Spackman, Anisotropic displacement parameters for H atoms using an ONIOM approach, Acta Crystallogr. Sect. B-Struct. Sci., 62, 875-888 (2006).

130. A. E. Whitten, D. Jayatilaka, and M. A. Spackman, Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data, J. Chem. Phys., 125(17) (2006).

131. A. E. Whitten, P. Turner, W. T. Klooster, R. O. Piltz and M. Spackman, Reassessment of large dipole moment enhancements in crystals: A detailed experimental and theoretical charge density analysis of 2-methyl-4-nitroaniline, J. Phys. Chem. A 110, 8763-8776 (2006).

132. G. J. Wilson, A. S. Matijasevich, D. R. G. Mitchell, J. C. Schulz, and G. D. Will, Modification of TiO_2 for enhanced surface properties: Finite Ostwald ripening by a microwave hydrothermal process, Langmuir, 22, 2016-2027 (2006).

133. E. L. S. Wong, T. C. Chilcott, M. James, and H. G. L. Coster, Electrical Impedance Spectroscopy Characterisations of Alkyl-Functionalised Si(111), Biophysical Reviews and Letters, 1(3), 301-307 (2006).

134. Q. Zhou, B. J. Kennedy and M. M. Elcombe, Neutron powder diffraction studies of $Ca_{2-x}Sr_xCoWO_6$ double perovskites, Physica B 385-386, 190-192 (2006).

135. Q. D. Zhou, B. J. Kennedy, and M. M. Elcombe, Synthesis and structural studies of cation-substituted Aurivillius phases $ASrBi_2Nb_2TiO_{12}$, J. Solid State Chem., 179(12), 3744-3750 (2006).

2007

1. M. Arora, B. J. Kennedy, C. G. Ryan, R. A. Boadle, D. M. Walker, C. L. Harland, B. Lai, Z. H. Cai, S. Vogt, H. Zoellner, and S. W. Y. Chan, The application of synchrotron radiation induced X-ray emission in the measurement of zinc and lead in Wistar rat ameloblasts, Arch. Oral Biol., 52(10), 938-944 (2007).

2. M. Avdeev, E. N. Caspi and S. Yakovlev, On the polyhedral volume ratios V_A/V_B in perovskites ABX_3, Acta Cryst. B 63, 363-372 (2007).

3. M. Avdeev, J. Jorgensen, S. Short, and R. B. Von Dreele, On the numerical corrections of time-of-flight neutron powder diffraction data, J. Appl. Crystallogr., 40, 710-715 (2007).

4. M. Avdeev, S. Yakovlev, A. A. Yaremchenko, and V. V. Kharton, Transitions between P2(1), P6(3)(root 3A), and P6(3)22 modifications of $SrAl_2O_4$ by in situ high-temperature X-ray and neutron diffraction, J. Solid State Chem., 180(12), 3535-3544 (2007).

5. T. Baikie, P. H. J. Mercier, M. M. Elcombe, J. Y. Kim, Y. Le Page, L. D. Mitchell, T. J. White, and P. S. Whitfield, Triclinic apatites, Acta Cryst. B 63, 251-256 (2007).

6. A. J. Berry, A. M. Walker, J. Hermann, H. S. O'Neill, G. J. Foran, and J. D. Gale, Titanium substitution mechanisms in forsterite, Chemical Geology, 242(1-2), 176-186 (2007).

7. S. K. Bhargava, D. B. Akolekar, and G. Foran, Investigations on gold nanoparticles supported on rare earth oxide catalytic materials, J. Mol. Catal. A-Chem., 267(1-2), 57-64 (2007).

8. R. Bircher, B. F. Abrahams, H. U. Guedel, and C. Boskovic, Synthesis, structure and magnetic properties of a novel Tb_4 Spin cluster and synthesis of a Tb chain, Polyhedron, 26(13), 3023-3028 (2007).

9. A. Blom, G. G. Warr, and A. Nelson, Structure of mixed DTAB/DDAB adsorbed layers on quartz - A neutron reflectometry and atomic force microscopy study, Colloid Surf. A-Physicochem. Eng. Asp., 310(1-3), 1-8 (2007).

10. M. D. Brown, B. M. Law, L. Marchand, L. B. Lurio, I. Kuzmenko, T. Gog, and W. A. Hamilton, X-ray and ellipsometric study of strong critical adsorption, Phys. Rev. E, 75(6), Art. No. 061606 (2007).

11. M. D. Brown, B. M. Law, S. Satija, W. A. Hamilton, E. Watkins, J. H. Cho and J. Majewski, Comparison of critical adsorption scaling functions obtained from neutron reflectometry and ellipsometry, J. Chem. Phys. 126, 204704-1 (2007).

12. J. Chan, A. E. Whitten, C. M. Jeffries, I. Bosanac, T. K. Mal, J. Ito, H. Porumb, T. Michikawa, K. Mikoshiba, J. Trewhella, and M. Ikura, Ligand-induced Conformational Changes via Flexible Linkers in the Amino-terminal region of the Inositol 1,4,5-Trisphosphate Receptor, Journal of Molecular Biology, 373(5), 1269-1280 (2007).

13. L. Chandra, C. E. Buckley, J. Connolly, L. Noren, G. Lockhart and E. Gilbert, Superstructure phase in the binary $C_{28}H_{58}$:$C_{36}H/D_{74}$ system, J. Appl. Crystallogr. 40, 51-55 (2007).

14. H. Chanvrier, I. A. M. Appelqvist, A. R. Bird, E. Gilbert, A. Htoon, Z. Li, P. J. Lillford, A. Lopez-Rubio, M. K. Morell, and D. L. Topping, Processing of Novel Elevated Amylose Wheats: Functional Properties and Starch Digestibility of Extruded Products, J. Agric. Food Chem., 55(25), 10248-10257 (2007).

15. H. Chanvrier, S. Uthayakumaran, I. A. M. Appelqvist, M. J. Gidley, E. P. Gilbert, and A. Lopez-Rubio, Influence of Storage Conditions on the Structure, Thermal Behavior, and Formation of Enzyme-Resistant Starch in Extruded Starches, J. Agric. Food Chem., 55(24), 9883-9890 (2007).

16. S. Ciampi, T. Bocking, K. A. Kilian, M. James, J. B. Harper, and J. J. Gooding, Functionalization of acetylene-terminated monolayers on Si(100) surfaces: A click chemistry approach, Langmuir, 23(18), 9320-9329 (2007).

17. W. B. Choi, L. Li, V. Luzin, R. Neiser, T. Gnaupel-Herold, H. J. Prask, S. Sampath, and A. Gouldstone, Integrated characterization of cold sprayed aluminum coatings, Acta Mater., 55(3), 857-866 (2007).

18. D. Comoletti, A. Grishaev, A. E. Whitten, I. Tsigelny, P. Taylor and J. Trewhella, Synaptic Arrangement of the Neuroligin/β-Neurexin Complex Revealed by X-Ray and Neutron Scattering, Structure 15, 693-705 (2007).

19. J. E. Daniels, T. R. Finlayson, A. J. Studer, M. Hoffmann and J. L. Jones,. Time-resolved diffraction measurements of electric-field-induced strain in tetragonal lead zirconate titanate, J. Appl. Phys. 101, 094104 (2007).

20. J. E. Daniels, T. R. Finlayson, M. Davis, D. Damjanovic, A. J. Studer, M. Hoffman and J. L. Jones, Neutron diffraction study of the polarization reversal mechanism in [111] c-oriented $Pb(Zn_{1/3}Nb_{2/3})O]$ - $xPbTiO_3$, J. Appl. Phys. 101, 104108 (2007).

21. S. A. Danilkin, G. Horton, R. Moore, G. Braoudakis and M. Hagen, The TAIPAN thermal triple-axis spectrometer at the OPAL Reactor, J. Neutron Res. 15, 55-60 (2007).

22. B. E. Etschmann, C. G. Ryan, S. Vogt, J. Maser, J. Brugger, C. L. Harland, and D. Legnini, Selective x-ray Bragg spectrometry: optimizing fluorescence microprobe sensitivity for precious metals, X-Ray Spectrom., 36, 111-121 (2007).

23. B. Finnigan, P. Casey, D. Cookson, P. Halley, K. Jack, R. Truss, and D. Martin, Impact of controlled particle size nanofillers on the mechanical properties of segmented polyurethane nanocomposites, Int. J. of Nanotechnology, 4(5), 496-515 (2007).

24. M. Gateshki, Q. Chen, L. M. Peng, P. Chupas, and V. Petkov, Structure of nanosized materials by high-energy X-ray diffraction study of titanate nanotubes, Z. Kristall., 222(11), 612-616 (2007).

25. M. Gateshki, J. M. Igartua, and A. Faik, Crystal structure and phase transitions of Sr_2CdWO_6, J. Solid State Chem., 180(8), 2248-2255 (2007).

26. M. Gateshki, M. Niederberger, A. S. Deshpande, Y. Ren and V. Petkov, Atomic-scale structure of nanocrystalline CeO_2-ZrO_2 oxides by total X-ray diffraction and pair distribution function analysis, J. Phys.: Condens. Matter 19, 156205 (2007).

27. M. Gateshki, S. Yin, Y. Ren, and V. Petkov, Titania polymorphs by soft chemistry: Is there a common structural pattern, Chem. Mat., 19(10), 2512-2518 (2007).

28. B. Gillon, A. Goujon, S. Willemin, J. Larionova, C. Desplanches, E. Ruiz, G. Andre, J. A. Stride, and C. Guerin, Neutron Diffraction and Theoretical DFT Studies of Two Dimensional Molecular-Based Magnet $K_2[Mn(H_2O)_2]3[Mo(CN)_7]_2{\bullet}6H_2O$, Inorg. Chem. 46, 1090 (2007).

29. R. Giulian, P. Kluth, B. Johannessen, L. L. Araujo, D. J. Llewellyn, D. J. Cookson, and M. C. Ridgway, Synthesis and characterization of ion-implanted Pt nanocrystals in SiO_2, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 257, 33-36 (2007).

30. C. Glover, J. McKinlay, M. Clift, B. Barg, J. Boldeman, M. Ridgway, G. Foran, R. Garret, P. Lay, and A. Broadbent, Status of the X-Ray Absorption Spectroscopy (XAS) Beamline at the Australian Synchrotron, AIP Conf. Proc., 882(1), 884-886 (2007)

31. M. D. Hall, C. K. Underwood, T. W. Failes, G. J. Foran, and T. W. Hambley, Using XANES to monitor the oxidation state of cobalt complexes, Aust. J. Chem., 60(3), 180-183 (2007).

32. T. L. Hanley, D. Sutton, E. Heeley, G. Moad and R. B. Knott, A Small Angle X-ray Scattering Study of the Effect of Chain Architecture on the Shear Induced Crystallisation of Branched and Linear Poly(ethylene terephthalate), J. Appl. Cryst. 40, s599-s604 (2007).

33. T. Hanley, D. Sutton, I. Karatchevtseva, D. Cookson, R. Burford, and R. Knott, Effects of selected process parameters on the morphology of poly(ethylene terephthalate) preforms and bottles, J. Appl. Polym. Sci., 106(1), 238-247 (2007).

34. S. J. Harker, T. J. Hicks, S. J. Kennedy, and D. H. Yu, High luminosity time of flight with polarisation analysis: $CeCu_6$, Physica B, 397(1-2), 15-19 (2007).

35. J. Healy, G. H. Edward, and R. B. Knott, Residual orientation in micro-injection molded parts, J. Appl. Crystallogr., 40, S393-S396 (2007).

36. J. W. Howarth, J. Meller, R. J. Solaro, J. Trewhella, and P. R. Rosevear, Phosphorylation-dependent conformational transition of the cardiac specific N-extension of troponin I in cardiac troponin, J. Mol. Biol., 373(3), 706-722 (2007).

37. N. Iqbal, N. H. van Dijk, S. E. Offerman, M. P. Moret, L. Katgerman, and G. J. Kearley, Nucleation kinetics during the solidification of aluminum alloys, Journal of Non-Crystalline Solids, 353(32-40), 3640-3643 (2007).

38. S. Jakani, T. Baudin, C. H. de Novion, and M. H. Mathon, Effect of impurities on the recrystallization texture in commercially pure copper-ETP wires,Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process., 456(1-2), 261-269 (2007).

39. M. James, M. Avdeev, P. Barnes, L. Morales, K. Wallwork, and R. Withers, Orthorhombic superstructures within the rare earth strontium-doped cobaltate perovskites: $Ln_{1-x}Sr_xCoO_{3-d}$ ($Ln = Y^{3+}$, Dy^{3+}, Yb3+; 0.750 <= x <= 0.875), J. Solid State Chem., 180(8), 2233-2247 (2007).

40. U. A. Jayasooriya, R. Grinter, P. L. Hubbard, G. M. Aston, J. A. Stride, G. A. Hopkins, L. Camus, I. D. Reid, S. P. Cottrell and S. F. J. Cox, Muon Implantation Studies Of Organometallics: Ferrocene, Eur. J. Chem. 13, 2266 (2007).

41. B. Johannessen, P. Kluth, R. Giulian, L. L. Araujo, D. J. Llewellyn, G. J. Foran, D. J. Cookson, and M. C. Ridgway, Modification of embedded Cu nanoparticles: Ion irradiation at room temperature, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 257, 37-41 (2007).

42. B. Johannessen, P. Kluth, D. J. Llewellyn, G. J. Foran, D. J. Cookson and M. C. Ridgway, Amorphization of embedded Cu nanocrystals by ion irradiation, Appl. Phys. Lett. 90, 7 (2007).

43. B. Johannessen, P. Kluth, D. J. Llewellyn, G. J. Foran, D. J. Cookson, and M. C. Ridgway, Ion-irradiation-induced amorphization of Cu nanoparticles embedded in SiO_2, Phys. Rev. B, 76(18) Art. No. 184203 (2007).

44. S. Y. Kamath, M. J. Arlen, W. A. Hamilton, and M. D. Dadmun, The dynamics of copolymers in homopolymer matrices, Eur. Phys. J.-Spec. Top., 141, 243-249 (2007).

45. S. J. Keough, T. L. Hanley, A. B. Wedding, and J. S. Quinton, Grazing incidence X-ray studies of ultra-thin Lumogen films, Surf. Sci., 601(24), 5744-5749 (2007).

46. V. V. Kharton, A. V. Kovalevsky, M. Avdeev, E. V. Tsipis, M. V. Patrakeev, A. A. Yaremchenko, E. N. Naumovich, and J. R. Frade, Chemically induced expansion of La_2NiO4_{+d} based materials, Chem. Mat. 19, 2027-2033 (2007).

47. N. Kirby, D. Cookson, C. Buckley, E. Bovell, and T. St Pierre, Iron K-edge anomalous small-angle X-ray scattering at 15-D-D at the Advanced Photon Source, J. Appl. Crystallogr., 40, S402-S407 (2007).

48. O. Kirstein, M. Prager, H. Grimm, A. Buchsteiner, and A. Wischnewski, Quasielastic neutron scattering experiments including activation energies and mathematical modeling of methyl halide dynamics, J. Chem. Phys., 127(9), Art. No. 094504 (2007).

49. O. Kirstein, M. I. Ripley, D. Tawfik, Strain scanning in Australia: Instrumentation and recent experiments, Mater. Sci. Forum 539-543, 2228-2233 (2007).

50. N. A. Klimenko, Y. V. Lisichkin, G. F. Syrykh, A. S. Ivanov, and J. A. Stride, Dispersion of acoustic-like and optic-like vibrational excitations in Ni_2B metallic glass, Crystallogr. Rep., 52(3), 471-473 (2007).

51. P. Kluth, B. Hoy, B. Johannessen, S. G. Dunn, G. J. Foran, and M. C. Ridgway, Formation and characterization of nanoparticles formed by sequential ion implantation of Au and Co into SiO_2, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 257, 80-84 (2007).

52. P. Kluth, B. Johannessen, R. Giulian, C. S. Schnohr, G. J. Foran, D. J. Cookson, A. P. Byrne, and M. C. Ridgway, Ion irradiation effects on metallic nanocrystals, Radiat. Eff. Defects Solids, 162(7-8), 501-513 (2007).

53. A. V. Kovalevsky, V. V. Kharton, A. A. Yaremchenko, Y. V. Pivak, E. V. Tsipis, S. O. Yakovlev, A. A. Markov, E. N. Naumovich, and J. R. Frade, Oxygen permeability, stability and electrochemical behavior of $Pr_2NiO_{4+delta}$-based materials, J. Electroceram., 18(3-4), 205-218 (2007).

54. O. Kruglova, E. Mendes, Z. Yildirim, M. Wuebbenhorst, F. M. Mulder, J. A. Stride, S. J. Picken, and G. J. Kearley, Structure and Dynamics of a Discotic Liquid-Crystalline Charge-Transfer Complex, Chem. Phys. Chem., 8(9), 1338-1344 (2007).

55. B. P. Ladewig, R. B. Knott, A. J. Hill, J. D. Riches, J. W. White, D. J. Martin, J. C. D. da Costa, and G. Q. Lu, Physical and electrochemical characterization of nanocomposite membranes of Nafion and functionalized silicon oxide, Chem. Mat., 19(9), 2372-2381 (2007).

56. B. P. Ladewig, R. B. Knott, D. J. Martin, J. C. D. da Costa, and G. Q. Lu, Nafion-MPMDMS nanocomposite membranes with low methanol permeability, Electrochem. Commun., 9(4), 781-786 (2007).

57. C. D. Ling, K. Aivazian, S. Schmid, and P. Jensen, Structural investigation of oxygen non-stoichiometry and cation doping in misfit-layered thermoelectric $(Ca_2CoO_{3-x})(CoO_2)$(delta), delta approximate to 1.61, J. Solid State Chem., 180(4), 1446-1455 (2007).

58. C. D. Ling, M. Avdeev, and K. Aivazian, Synthesis, structure, and stability of the hightemperature 6H-type perovskite phase $Ba_3BaSb_2O_9$, Acta Crystallogr. Sect. B-Struct. Sci., 63, 584-588 (2007).

59. K. -D. Liss, A. Bartels, H. Clemens, S. Bystrzanowski, A. Stark, T. Buslaps, F. P. Schimansky, R. Gerling and A. Schreyer, A Study of Recrystallization and Phase Transitions in Intermetallic Titanium Aluminides by In-Situ High-Energy X-Ray Diffraction, Mater. Sci. Forum 539-543, 1519-1524 (2007).

60. Y. Liu, C. M. Brown, D. A. Neumann, V. K. Peterson, and C. J. Kepert, Inelastic neutron scattering of H_2 adsorbed in HKUST-1, J. Alloy. Compd., 446-447, 385-388 (2007).

61. W. H. Liu, B. Etschmann, G. Foran, M. Shelley, and J. Brugger, Deriving formation constants for aqueous metal complexes from XANES spectra: Zn^{2+} and Fe^{2+} chloride complexes in hypersaline solutions, Am. Miner., 92(5-6), 761-770 (2007).

62. A. Lopez-Rubio, A. Htoon & E.P. Gilbert, The influence of extrusion and digestion on the nanostructure of high-amylose maize starch, Biomacromolecules 8, 1564-1572 (2007).

63. V. Luca, M. G. Blackford, K. S. Finnie, P. J. Evans, M. James, M. J. Lindsay, M. Skyllas-Kazacos, and P. R. F. Barnes, Sol-gel tungsten oxide/titanium oxide multilayer nanoheterostructured thin films: Structural and photoelectrochemical properties, J. Phys. Chem. C, 111(50), 18479-18492 (2007)

64. M. E. Manley, M. Yethiraj, H. Sinn, H. M. Volz, A. Alatas, J. C. Lashley, W. L. Hults, G. H. Lander, D. J. Thoma, and J. L. Smith, Intrinsically localized vibrations and the mechanical properties of alpha-uranium, J. Alloy. Compd., 444, 129-132 (2007).

65. R. J. McQueeney, M. Yethiraj, S. Chang, W. Montfrooij, T. G. Perring, J. M. Honig, and P. Metcalf, Zener double exchange from local valence fluctuations in magnetite, Phys. Rev. Lett., 99(24), Art. No. 246401 (2007).

66. F. Merzel, F. Fontaine-Vive, M. R. Johnson, and G. J. Kearley, Atomistic model of DNA: Phonons and base-pair opening, Phys. Rev. E, 76(3), 031917-5 (2007).

67. W. Montfrooij, J. Lamsal, M. Aronson, M. Bennett, A. de Visser, H. Y. Kai, N. T. Huy, M. Yethiraj, M. Lumsden, and Y. M. Qiu, Ground state of a quantum critical system: Neutron scattering on $Ce(Ru_{1-x}Fex)_2Ge_2$, Phys. Rev. B, 76(5), Art. No. 052404 (2007).

68. B. W. Muir, A. Nelson, A. Fairbrother, C. Fong, P. G Hartley, M. James and K. M. McLean, A comparative X-ray and neutron reflectometry study of reactive amine containing plasma polymer films, Plasma Processes and Polymers 4, 433-444 (2007).

69. A. M. Mulders, U. Staub, V. Scagnoli, Y. Tanaka, A. Kikkawa, K. Katsumata and J. M. Tonnerre, Manipulating 4f quadrupolar pair-interactions in TbB_2C_2 using a magnetic field, Phys. Rev. B 75, 184438 (2007).

70. P. Muller-Buschbaum, E. Bauer, E. Maurer, A. Nelson, and R. Cubitt, In-situ neutron reflectometry probing competitive swelling and de-swelling of thin polystyrene films, Phys. Status Solidi-Rapid Res. Lett. 1, R68-R70 (2007).

71. N. Nishiyama, Y. Wang, M. L. Rivers, S. R. Sutton, and D. Cookson, Rheology of epsilon-iron up to 19 GPa and 600 K in the D-DIA, Geophys. Res. Lett., 35(23) Art. No. L23304 (2007).

72. H. B. Nguyen, L. Noren, Y. Liu, R. L. Withers, X. Y. Wei, and M. M. Elcombe, The disordered structures and low temperature dielectric relaxation properties of two misplaced-displacive cubic pyrochlores found in the Bi_2O_3-(MO)-O-II-Nb_2O_5 (M = Mg, Ni) systems, J. Solid State Chem., 180(9), 2558-2565 (2007).

73. J. Overgaard, M. P. Waller, R. Piltz, J. A. Platts, P. Emseis, P. Leverett, P. A. Williams, and D. E. Hibbs, Experimental and theoretical charge density distribution in two ternary cobalt(III) complexes of aromatic amino acids, J. Phys. Chem. A, 111(40), 10123-10133 (2007).

74. H. B. Park, C. H. Jung, Y. M. Lee, A. J. Hill, S. J. Pas, S. T. Mudie, E. Van Wagner, B. D. Freeman, and D. J. Cookson, Polymers with cavities tuned for fast selective transport of small molecules and ions, Science, 318(5848), 254-258 (2007).

75. M. J. Park, K. H. Downing, A. Jackson, E. D. Gomez, A. M. Minor, D. Cookson, A. Z. Weber, and N. P. Balsara, Increased water retention in polymer electrolyte membranes at elevated temperatures assisted by capillary condensation, Nano Lett., 7(11), 3547-3552 (2007).

76. V. Peterson, Y. Liu, C. M. Brown, and C. J. Kepert, Structural Characterization of D_2 in Cu_3(1,3,5-benzenetricarboxylate)$_2$ Using Neutron Powder Diffraction, Mat. Sci. For., 561-565, 1601-1604 (2007).

77. S. K. Pradhan, M. Gateshki, M. Niederberger, Y. Ren, and V. Petkov, $PbZr_{1-x}Ti_xO_3$ by soft synthesis: Structural aspects, Phys. Rev. B, 76(1), Art. No. 014114 (2007).

78. V. Renken, D. H. Yu, and M. Donath, Quantum-well states and spin polarization in thin Ni films on Cu(001), Surf. Sci., 601(24), 5770-5774 (2007).

79. D. M. Rodriguez, F. Plazaola, J. S. Garitaonandia, and G. J. Cuello, Structural study of the re-entrant spin-glass behaviour of Fe-Al alloys, J. Magn. Magn. Mater., 316(2), E488-E491 (2007).

80. D. M. Rodriguez, D. S. Schmool, J. S. Garitaonandia, and F. Plazaola, Ferromagnetic resonance study of Fe rich Fe-Al intermetallic alloys, J. Magn. Magn. Mater., 316(2), E484-E487 (2007).

81. J. L. Ruggles, K. M. Baldwin, S. A. Holt, G. J. Foran, and I. R. Gentle, Rigid films of an anionic porphyrin and a dialkyl chain surfactant, J. Phys. Chem. B, 111(20), 5651-5657 (2007).

82. K. C. Rule, G. J. McIntyre, S. J. Kennedy, and T. J. Hicks, Single-crystal and powder neutron diffraction experiments on $FePS_3$: Search for the magnetic structure, Phys. Rev. B, 76(13) (2007).

83. P. J. Saines, J. R. Spencer, B. J. Kennedy, and M. Avdeev, Structures and crystal chemistry of the double perovskites $Ba_2LnB'O_6$ (Ln = lanthanide B' = Nb^{5+} and Ta^{5+}): Part I. Investigation of Ba_2LnTaO_6 using synchrotron X-ray and neutron powder diffraction, J. Solid State Chem., 180(11), 2991-3000 (2007).

84. P. J. Saines, B. J. Kennedy and M. M. Elcombe, Structural phase transitions and crystal chemistry of the series Ba_2LnBO_6 (Ln = lanthanide and B = Nb^{5+} or Sb^{5+}), J. Solid State Chem. 180, 401-409 (2007).

85. P. S. Salamakha, O. L. Sologub, J. R. Hester, C. Rizzoli, A. P. Goncalves, and M. Almeida, Rietveld refinement of the RNi_4B compounds (R = Gd, Tb, Er), J. Alloy. Compd., 439(1-2), 162-165 (2007).

86. C. S. Schnohr, P. Kluth, A. P. Byrne, G. J. Foran, and M. C. Ridgway, EXAFS study of the amorphous phase of InP after swift heavy ion irradiation,Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 257, 293-296 (2007).

87. N. Sharma, C. D. Ling, G. E. Wrighter, P. Y. Chen, B. J. Kennedy and P. L. Lee, Three-layer Aurivillius phases containing magnetic transition metal cations: $Bi_{2-x}Sr_{2+x}(Nb,Ta)_{2+x}M_{1-x}O_{12}$, M = $Ru^{4+}Ir^{4+}$. Mn^{4+}, x approximate to 0.5, J. Solid State Chem. 180, 370-376 (2007).

88. M. Singh, O. Odusanya, G. M. Wilmes, H. B. Eitouni, E. D. Gomez, A. J. Patel, V. L. Chen, M. J. Park, P. Fragouli, H. Iatrou, N. Hadjichristidis, D. Cookson, and N. P. Balsara, Effect of molecular weight on the mechanical and electrical properties of block copolymer electrolytes, Macromolecules, 40(13), 4578-4585 (2007).

89. P. Starck, W. K. J. Mosse, N. J. Nicholas, M. Spiniello, J. Tyrrell, A. Nelson, G. G. Qiao, and W. A. Ducker, Surface chemistry and rheology of polysulfobetaine-coated silica, Langmuir, 23(14), 7587-7593 (2007).

90. U. Staub, M. Garcia-Fernandez, A. M. Mulders, Y. Bodenthin, M. J. Martinez-Lope, and J. A. Alonso, Soft x-ray resonant magnetic powder diffraction on $PrNiO_3$, J. Phys.: Condens. Matter, 19, 9 (2007).

91. J. R. Stewart, K. H. Andersen, J. A. Stride, H. Mutka and H. Schober, The assets of Crystal Monochromator-Fermi Chopper Time-of-Flight on Continuous Sources - Potential for High Efficiency PASTIS Operation, J. Neutron Res. 15, 95-104 (2007).

92. G. F. Syrykh, M. G. Zemlyanov, A. S. Ivanov, J. A. Stride, Y. V. Lisichkin, and N. A. Khmenko, Observation of the collective vibrational modes in $Ni_{42}Nb_{58}$ metallic glass, J. Non-Cryst. Solids, 353(32-40), 3188-3191 (2007).

93. D. Tawfik, P. J. Mutton, O. Kirstein, and W. K. Chiu, A comparative study between FEA, trepanning and neutron strain diffraction on residual stresses in flash-butt welded rails, J. Neutron Res., 15(3), 199 - 205 (2007).

94. J. van Lierop, B. W. Southern, K. W. Lin, Z. Y. Guo, C. L. Harland, R. A. Rosenberg, and J. W. Freeland, Exchange bias in a columnar nanocrystalline $Ni_{80}Fe_{20}$/CoO thin film, Phys. Rev. B, 76(22), Art. No. 224432 (2007).

95. M. Wagemaker, W. J. H. Borghols, E. R. H. van Eck, A. P. M. Kentgens, G. J. Kearley, and F. M. Mulder, The Influence of Size on Phase Morphology and Li-Ion Mobility in Nanosized Lithiated Anatase TiO_2, Chem. Eur. J., 13(7), 2023-2028 (2007).

96. O. Waldmann, R. Bircher, G. Carver, A. Sieber, H. U. Gudel, and H. Mutka, Exchange-coupling constants, spin density map, and Q dependence of the inelastic neutron scattering intensity in single-molecule magnets, Phys. Rev. B, 75(17) (2007).

97. N. A. S. Webster, C. D. Ling, C. L. Raston, and F. J. Lincoln, The structure and conductivity of new fluorite-type Bi_2O_3-Er_2O_3-PbO materials, Solid State Ion., 178(25-26), 1451-1457 (2007)

98. E. Whitten, D. A. Jacques, B. Hammouda, T. Hanley, G. F. King, J. M. Guss, J. Trewhella and D. B. Langley, The Structure of the KinA-Sda Complex Suggests an Allosteric Mechanism of Histidine Kinase Inhibition, J. Molec. Biology 368, 407-420 (2007).

99. E. L. S. Wong, M. James, T. C. Chilcott, and H. G. L. Coster, Characterisation of alkyl-functionalised Si(111) using reflectometry and AC impedance spectroscopy, Surf. Sci., 601(24), 5740-5743 (2007).

100. R. C. Woodward, J. Heeris, T. G. St.Pierre, M. Saunders, E. P. Gilbert, M. Rutnakornpituk, Q. Zhang and J. S. Riffle, Measurement of Particle Size Distribution of Magnetic Nanoparticles, J. Appl. Cryst. 40, s495-s500 (2007).

101. S. Yakovlev, V. Kharton, A. Yaremchenko, A. Kovalevsky, E. Naumovich, and J. Frade, Mixed conductivity, thermal expansion and defect chemistry of A-site deficient $LaNi_{0.5}Ti_{0.5}O_{3-d}$, J. Eur. Ceram. Soc., 27(13-15), 4279-4282 (2007).

102. A. Yaremehenko, V. V. Kharton, M. Avdeev, A. L. Shaula, and F. M. B. Marques, Oxygen permeability, thermal expansion and stability of $SrCo_{0.8}Fe_{0.2}O_{3-d}SrAl_2O_4$ Composites, Solid State Ion., 178(19-20), 1205-1217 (2007).

103. L. A. Yeoh, K. D. Liss, A. Bartels, H. Chladil, M. Avdeev, H. Clemens, R. Gerling, and T. Buslaps, In situ high-energy X-ray diffraction study and quantitative phase analysis in the alpha plus gamma phase field of titanium aluminides, Scr. Mater., 57(12), 1145-1148 (2007).

104. D. H. Yu, M. R. Fitzsimmons, E. P. Gilbert, R. C. Woodward, S. H. Kilcoyne, and R. A. Robinson, Neutron depolarization studies of Pd-Ni-Fe-P alloy, Physica B, 397(1-2), 30-32 (2007).

105. D. H. Yu, C. Math, M. Meier, M. Escher, G. Rangelov, and M. Donath, Characterisation and application of a SPLEED-based spin polarisation analyser, Surf. Sci., 601(24), 5803-5808 (2007).

106. H. Zhang, R. N. Lamb, and D. J. Cookson, Nanowetting of rough superhydrophobic surfaces, Appl. Phys. Lett., 91(25), Art. No 254106 (2007).

107. Q. D. Zhou, B. J. Kennedy and M. M. Elcombe, Composition and temperature dependent phase transitions in Co-W double perovskites, a synchrotron X-ray and neutron powder diffraction study, J. Solid State Chem. 180, 541-548 (2007).

108. Q. D. Zhou, B. J. Kennedy, M. M. Elcombe, and R. L. Withers, Composition- and temperature-dependent phase transitions in 1:3 ordered perovskites $Ba_{4-x}Sr_xNaSb_3O_{12}$, J. Solid State Chem., 180(11), 3082-3092 (2007).

2008

1. L. M. Anovitzi, G. W. Lynn, D. R. Cole, G. Rother, L. F. Allard, W. A. Hamilton, L. Porcar, and M. H. Kim, A new approach to quantification of metamorphism using ultra-small and small angle neutron scattering, Geochim. Cosmochim. Acta, 72(12), A28-A28 (2008).
2. L. L. Araujo, G. J. Foran, and M. C. Ridgway, Multiple scattering effects on the EXAFS of Ge nanocrystals, J. Phys.-Condes. Matter, 20(16), Art. No. 165210 (2008).
3. L. L. Araujo, R. Giulian, B. Johannessen, D. J. Llewellyn, P. Kluth, G. D. Azevedo, D. J. Cookson, and M. C. Ridgway, Structural characterization of Ge nanocrystals in silica amorphised by ion irradiation, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 266(12-13), 3153-3157 (2008).
4. L. L. Araujo, R. Giulian, D. J. Sprouster, C. S. Schnohr, D. J. Llewellyn, P. Kluth, D. J. Cookson, G. J. Foran, and M. C. Ridgway, Size-dependent characterization of embedded Ge nanocrystals: Structural and thermal properties, Phys. Rev. B, 78(9), 15 (2008).
5. J. Berry, H. S. C. O'Neill, and G. J. Foran, The oxidation state of Uranium in mantle melts, Geochim. Cosmochim. Acta, 72(12), A79-A79 (2008).
6. K. F. Cai, X. R. He, M. Avdeev, D. H. Yu, J. L. Cui, and H. Li, Preparation and thermoelectric properties of $AgPb_mSbSe_{m+2}$ materials, J. Solid State Chem., 181(6), 1434-1438 (2008).
7. G. Chen, W. H. Yu, D. Singh, D. Cookson, and J. Routbort, Application of SAXS to the study of particle-size-dependent thermal conductivity in silica nanofluids, J. Nanopart. Res., 10(7), 1109-1114 (2008).
8. J. H. J. Cho, G. S. Smith, W. A. Hamilton, D. J. Mulder, T. L. Kuhl, and J. Mays, Surface force confinement cell for neutron reflectometry studies of complex fluids under nanoconfinement, Rev. Sci. Instrum., 79(10), 7 (2008).
9. M. Choucair, P. Thordarson and J. A. Stride, Gram-scale production of graphene based on solvothermal synthesis and sonication, Nature Nanotechnology, (2008)
10. H. Clemens, H. F. Chladil, W. Wallgram, G. A. Zickler, R. Gerling, K. D. Liss, S. Kremmer, V. Guther, and W. Smarslyg, In and ex situ investigations of the beta-phase in a Nb and Mo containing gamma-TiAl based alloy, Intermetallics, 16(6), 827-833 (2008).
11. N. P. Cowieson, G. King, D. Cookson, I. Ross, T. Huber, D. A. Hume, B. Kobe, and J. L. Martin, Cortactin adopts a globular conformation and bundles actin into sheets, J. Biol. Chem., 283(23), 16187-16193 (2008).
12. R. De Marco, J. P. Veder, G. Clarke, A. Nelson, K. Prince, E. Pretsch, and E. Bakker, Evidence of a water layer in solid-contact polymeric ion sensors, Phys. Chem. Chem. Phys., 10(1), 73-76 (2008).
13. F. Demmel, G. Heusel, I. Waldner, J. Stride, and H. Bertagnolli, Collective High Frequency Motions in Liquid Deuterium Fluoride, Z. Phys. Chemie-Int. J. Res. Phys. Chem. Chem. Phys., 222(10), 1551-1558 (2008).
14. Y. D. Dong, A. W. Dong, I. Larson, M. Rappolt, H. Amenitsch, T. Hanley, and B. J. Boyd, Impurities in commercial phytantriol significantly alter its lyotropic liquid-crystalline phase behavior, Langmuir, 24(13), 6998-7003 (2008).
15. Faik, M. Gateshki, J. M. Igartua, J. L. Pizarro, M. Insausti, R. Kaindl, and A. Grzechnik, Crystal structures and cation ordering of Sr_2AlSbO_6 and Sr_2CoSbO_6, J. Solid State Chem., 181(8), 1759-1766 (2008).
16. M. Garcia-Fernandez, V. Scaunoli, U. Staub, A. M. Mulders, M. Janousch, Y. Bodenthin, D. Meister, B. D. Patterson, A. Mirone, Y. Tanaka, T. Nakamura, S. Grenier, Y. Huang, and K. Conder, Magnetic and electronic Co states in the layered cobaltate $GdBaCo_2O_{5.5-x}$, Phys. Rev. B, 78(5), 13 (2008).
17. M. Gateshki, L. Suescun, S. Kolesnik, J. Mais, K. Swierczek, S. Short, and B. Dabrowski, Structural, magnetic and electronic properties of $LaNi_{0.5}Fe_{0.5}O_3$ in the temperature range 5-1000 K, J. Solid State Chem., 181(8), 1833-1839 (2008).
18. M. D. W. Griffin, R. C. J. Dobson, F. G. Pearce, L. Antonio, A. E. Whitten, K. Liew, J. P. Mackay, J. Trewhella, G. B. Jameson, M. A. Perugini, and J. A. Gerrard, Evolution of quaternary structure in a homotetrameric enzyme, J. Mol. Biol., 380(4), 691-703 (2008).
19. Grishaev, V. Tugarinov, L. E. Kay, J. Trewhella, and A. Bax, Refined solution structure of the 82-kDa enzyme malate synthase G from joint NMR and synchrotron SAXS restraints, J. Biomol. NMR, 40(2), 95-106 (2008).
20. M. Garcia-Fernandez, U. Staub, Y. Bodenthin, S. M. Lawrence, A. M. Mulders, C. E. Buckley, S. Weyeneth, E. Pomjakushina, and K. Conder, Resonant soft x-ray powder diffraction study to determine the orbital ordering in A-site-ordered $SmBaMn_2O_6$, Phys. Rev. B, 77(6), Art. No. 060402 (2008).
21. C. Glover, J. McKinlay, M. Clift, B. Barg, J. Boldeman, M. Ridgway, G. Foran, R. Garret, P. Lay, and A. Broadbent, Status of the X-Ray Absorption Spectroscopy (XAS) Beamline at the Australian Synchrotron, AIP Conf. Proc., 882(1), 884-886 (2007).
22. R. Giulian, P. Kluth, L. L. Araujo, D. J. Sprouster, A. P. Byrne, D. J. Cookson, and M. C. Ridgway, Shape transformation of Pt nanoparticles induced by swift heavy-ion irradiation, Phys. Rev. B, 78(12), 8 (2008).
23. D. A. Jacques, D. B. Langley, C. M. Jeffries, K. A. Cunningham, W. F. Burkholder, J. M. Guss, and J. Trewhella, Histidine Kinase Regulation by a Cyclophilin-like Inhibitor, J. Mol. Biol., 384(2), 422-435 (2008).
24. C. M. Jeffries, A. E. Whitten, S. P. Harris, and J. Trewhella, Small-angle X-ray scattering reveals the N-terminal domain organization of cardiac myosin binding protein C, J. Mol. Biol., 377(4), 1186-1199 (2008).
25. S. Y. Kamath, M. J. Arlen, W. A. Hamilton, and M. D. Dadmun, The importance of thermodynamic interactions on the dynamics of multicomponent polymer systems revealed by examination of the dynamics of copolymer/homopolymer blends, Macromolecules, 41(9), 3339-3348 (2008).
26. Karatchevtseva, A. Heinemann, V. Hartley, and R. Knott, Structure of Organic-Inorganic Nanohybrids Incorporating Titanium(IV) Oxoalkoxyacylate Nanoclusters: A SANS Study, J. Phys. Chem. B, 112(51), 16478-16484 (2008).
27. H. Kawano-Furukawa, S. Ohira-Kawamura, H. Tsukagoshi, C. Kobayashi, T. Nagata, N. Sakiyama, H. Yoshizawa, M. Yethiraj, J. Suzuki, and H. Takeya, Flux Line Lattice Structure in YNi_2B_2C, J. Phys. Soc. Jpn., 77(10), 5 (2008).
28. C. S. Kealley, M. M. Elcombe, R. Wuhrer, and E. P. Gilbert, Application of small-angle scattering to study the effects of moisture content on a native soy protein, J. Appl. Crystallogr., 41, 628-633 (2008).
29. C. S. Kealley, M. M. Elcombe, and A. van Riessen, Microstrain in hydroxyapatite carbon nanotube composites, J. Synchrot. Radiat., 15, 86-90 (2008).
30. C. S. Kealley, B. A. Latella, A. van Riessen, M. M. Elcombe, and B. Ben-Nissan, Micro- and Nano-Indentation of a Hydroxyapatite-Carbon Nanotube Composite, J. Nanosci. Nanotechnol., 8(8), 3936-3941 (2008).
31. C. S. Kealley, M. K. Rout, M. R. Dezfouli, E. Strounina, A. K. Whittaker, I. A. M. Appelqvist, P. J. Lillford, E. P. Gilbert, and M. J. Gidley, Structure and Molecular Mobility of Soy Glycinin in the Solid State, Biomacromolecules, 9(10), 2937-2946 (2008).

32. V. V. Kharton, E. V. Tsipis, V. A. Kolotygin, M. Avdeev, A. P. Viskup, J. C. Waerenborgh, and J. R. Frade, Mixed conductivity and stability of $CaFe_2O_{4-delta}$, J. Electrochem. Soc., 155(3), P13-P20 (2008).

33. W. T. Klooster, R. O. Piltz, and E. R. T. Tiekink, Crystal and molecular structure of dichloro(1,10-phenanthroline) dimethyltin(IV), Me_2Sn(1,10-phenanthroline)Cl2, determined by neutron diffraction, Z. Kristallogr., 223(9), 598-601 (2008).

34. P. Kluth, C. S. Schnohr, D. J. Sprouster, A. P. Byrne, D. J. Cookson, and M. C. Ridgway, Measurement of latent tracks in amorphous SiO_2 using small angle X-ray scattering, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms, 266(12-13), 2994-2997 (2008).

35. Li, D. J. Cookson, and A. R. Gerson, Crystal growth through progressive densification identified by synchrotron small-angle X-ray scattering, Cryst. Growth Des., 8(5), 1730-1733 (2008).

36. K.-D. Liss, A. Stark, A. Bartels, H. Clemens, T. Buslaps, D. Phelan, and L. A. Yeoh, Directional Atomic Rearrangements During Transformations between the alpha- and gamma-Phases in Titanium Aluminides, Adv. Eng. Mater., 10(4), 389-392 (2008).

37. M. Lonescu, N. P. Bhatia, D. D. Cohen, A. Kachenko, R. Siegele, M. A. Marcus, S. Fakra, and G. Foran, X-ray absorption spectroscopy at the Ni-K edge in Stackhousia tryonii Bailey hyperaccumulator, X-Ray Spectrom., 37(6), 629-634 (2008).

38. Lopez-Rubio, B. M. Flanagan, E. P. Gilbert, and M. J. Gidley, A novel approach for calculating starch crystallinity and its correlation with double helix content: A combined XRD and NMR study, Biopolymers, 89(9), 761-768 (2008).

39. Lopez-Rubio, B. M. Flanagan, A. K. Shrestha, M. J. Gidley, and E. P. Gilbert, Molecular rearrangement of starch during in vitro digestion: Toward a better understanding of enzyme resistant starch formation in processed starches, Biomacromolecules, 9(7), 1951-1958 (2008).

40. D. Lott, J. Fenske, A. Schreyer, P. Mani, G. J. Mankey, F. Klose, W. Schmidt, K. Schmalzl, and E. V. Tartakovskaya, Antiferromagnetism in a $Fe_{50}Pt_{40}Rh_{10}$ thin film investigated using neutron diffraction, Phys. Rev. B, 78(17), 174413-10 (2008).

41. D. Lott, F. Klose, H. Ambaye, G. J. Mankey, P. Mani, M. Wolff, A. Schreyer, H. M. Christen, and B. C. Sales, Chemical-order-induced magnetic exchange bias in epitaxial $FePt_3$ films, Phys. Rev. B, 77(13), Art. No. 132404 (2008).

42. V. Luca, W. K. Bertram, G. D. Sizgek, B. Yang, and D. Cookson, Delineating the first few seconds of supramolecular self-assembly of mesostructured titanium oxide thin films through time-resolved small angle X-ray scattering, Langmuir, 24(19), 10737-10745 (2008).

43. N. Magnani, A. Paoluzi, L. Pareti, and J. A. Stride, Inelastic neutron scattering study of $Pr_2Co_{12}Fe_5$, J. Phys.-Condes. Matter, 20(10), Art. No. 104222 (2008).

44. Manoun, J. M. Igartua, M. Gateshki, and S. K. Saxena, High-pressure study of the Sr_2CoWO_6 ordered double perovskite tungstate oxide, J. Mol. Struct., 888(1-3), 244-252 (2008).

45. R. J. McQueeney, S. O. Diallo, V. P. Antropov, G. D. Samolyuk, C. Broholm, N. Ni, S. Nandi, M. Yethiraj, J. L. Zarestky, J. J. Pulikkotil, A. Kreyssig, M. D. Lumsden, B. N. Harmon, P. C. Canfield, and A. I. Goldman, Anisotropic Three-Dimensional Magnetism in $CaFe_2As_2$, Phys. Rev. Lett., 101, Art. No. 227205 (2008)

46. M. K. Mistry, N. R. Choudhury, N. K. Dutta, R. Knott, Z. Q. Shi, and S. Holdcroft, Novel Organic-Inorganic Hybrids with Increased Water Retention for Elevated Temperature Proton Exchange Membrane Application, Chem. Mat., 20(21), 6857-6870 (2008).

47. R. A. Mole, S. P. Cottrell, J. A. Stride, and P. T. Wood, Muon spin relaxation study of manganese hydroxy squarate, Inorg. Chim. Acta, 361(12-13), 3718-3722 (2008).

48. F. M. Mulder, T. J. Dingemans, H. G. Schimmel, A. J. Ramirez-Cuesta, and G. J. Kearley, Hydrogen adsorption strength and sites in the metal organic framework MOF5: Comparing experiment and model calculations, Chem. Phys., 351(1-3), 72-76 (2008).

49. F. M. Mulder, M. Wagemaker, L. van Eijck, and G. J. Kearley, Hydrogen in porous tetrahydrofuran clathrate hydrate, ChemPhysChem, 9(9), 1331-1337 (2008).

50. S. T. Ochsenbein, F. Tuna, M. Rancan, R. S. G. Davies, C. A. Muryn, O. Waldmann, R. Bircher, A. Sieber, G. Carver, H. Mutka, F. Fernandez-Alonso, A. Podlesnyak, L. P. Engelhardt, G. A. Timco, H. U. Gudel, and R. E. P. Winpenny, Studies of finite molecular chains: Synthesis, structural, magnetic and inelastic neutron scattering studies of hexa- and heptanuclear chromium horseshoes, Chem.-Eur. J., 14(17), 5144-5158 (2008).

51. S. R. Olsen, S. J. Kennedy, S. Kim, J. C. Schulz, R. Thiering, E. P. Gilbert, W. Lu, M. James, and R. A. Robinson, Novel Cryogenic Engineering Solutions for the New Australian Research Reactor OPAL, AIP Conference Proceedings, 985(1), 299-306 (2008).

52. M. J. Park, A. J. Nedoma, P. L. Geissler, N. P. Balsara, A. Jackson, and D. Cookson, Humidity-induced phase transitions in ion-containing block copolymer membranes, Macromolecules, 41(6), 2271-2277 (2008).

53. V. K. Peterson, P. E. Stutzman, and R. A. Livingston, Microscopic investigation of modified hydration kinetics in tricalcium silicate paste and mortar strength caused by dicalcium silicate addition, J. Mater. Res., 23(4), 1015-1019 (2008).

54. S. Pojprapai (Imlao), J. L. Jones, A. J. Studer, J. Russell, N. Valanoor, and M. Hoffman, Ferroelastic domain switching fatigue in lead zirconate titanate ceramics, Acta Mater., 56(7), 1577-1587 (2008).

55. S. K. Poznyak, V. V. Kharton, J. R. Frade, A. A. Yaremchenko, E. V. Tsipis, S. O. Yakovlev, and I. P. Marozau, Behavior of $(La,Sr)CoO_3$- and La_2NiO_4-based ceramic anodes in alkaline media: Compositional and microstructural factors, J. Solid State Electrochem., 12(1), 15-30 (2008).

56. Prescimone, C. J. Milios, S. Moggach, J. E. Warren, A. R. Lennie, J. Sanchez-Benitez, K. Kamenev, R. Bircher, M. Murrie, S. Parsons, and E. K. Brechin, Mn-6 under pressure: A combined crystallographic and magnetic study, Angew. Chem.-Int. Edit., 47(15), 2828-2831 (2008).

57. S. A. Pullen, E. P. Gilbert, S. R. Olsen, E. A. Lang, and K. R. Doolan, An in situ rapid heat-quench cell for small-angle neutron scattering, Meas. Sci. Technol., 19, Art. No. 065707 (2008).

58. Rowda, M. Avdeev, P. L. Lee, P. F. Henry, and C. D. Ling, Structures of 6H perovskites $Ba_3CaSb_2O_9$ and $Ba_3SrSb_2O_9$ determined by synchrotron X-ray diffraction, neutron powder diffraction and ab initio calculations, Acta Crystallogr. Sect. B-Struct. Sci., 64, 154-159 (2008).

59. P.J. Saines, B. J. Kennedy, M. M. Elcombe, H. H. Harris, L. Y. Jang and Z. Zhang, Phase and Valence Transitions in $Ba_2LnSn_xSb_{1-x}O_{6-\delta}$ (Ln = Pr, Tb). J. Solid State Chem. 181(11) 2941-2952, (2008)

60. V. Scagnoli, U. Staub, Y. Bodenthin, M. Garcia-Fernandez, A. M. Mulders, G. I. Meijer, and G. Hammerl, Induced noncollinear magnetic order of Nd^{3+} in $NdNiO_3$ observed by resonant soft x-ray diffraction, Phys. Rev. B, 77(11), Art. No. 115138 (2008).

61. S. Schnohr, L. L. Araujo, P. Kluth, D. J. Sprouster, G. J. Foran, and M. C. Ridgway, Atomic-scale structure of $Ga_{1-x}In_xP$ alloys measured with extended x-ray absorption fine structure spectroscopy, Phys. Rev. B, 78(11), 8 (2008).

62. C. S. Schnohr, P. Kluth, A. P. Byrne, G. J. Foran, and M. C. Ridgway, Comparison of the atomic structure of InP amorphized by electronic or nuclear ion energy-loss processes, Phys. Rev. B, 77(7), Art. No. 073204 (2008).

63. N. Sharma, B. Kennedy, M. Elcombe, Y. Liu, and C. D. Ling, Coexistence of ferroelectricity and magnetism in transition-metal-doped n = 3 Aurivillius phases, J. Phys.: Condens. Matter, 20(2), 025215 (2008).

64. U. Staub, V. Scagnoli, Y. Bodenthin, M. Garcia-Fernandez, R. Wetter, A. M. Mulders, H. Grimmer, and M. Horisberger, Polarization analysis in soft X-ray diffraction to study magnetic and orbital ordering, J. Synchrot. Radiat., 15(469-476 (2008).

65. Stercel, T. Egami, H. A. Mook, M. Yethiraj, J. H. Chung, M. Arai, C. Frost, and F. Dogan, Composition dependence of the in-plane Cu-O bond-stretching LO phonon mode in $YBa_2Cu_3O_{6+x}$, Phys. Rev. B, 77(1), Art. No. 014502 (2008).

66. F. Syrykh, A. S. Ivanov, N. A. Klimenko, Y. V. Lisichkin, H. Mutka, and J. A. Stride, Propagating vibrational modes in the Zr-Be metallic glasses, J. Phys.-Condes. Matter, 20(10), Art. No. 104241 (2008).

67. M. Taraban, H. Zhan, A. E. Whitten, D. B. Langley, K. S. Matthews, L. Swint-Kruse, and J. Trewhella, Ligand-induced conformational changes and conformational dynamics in the solution structure of the lactose repressor protein, J. Mol. Biol., 376(2), 466-481 (2008).

68. S. C. M. Teixeira, G. Zaccai, J. Ankner, M. C. Bellissent-Funel, R. Bewley, M. P. Blakeley, P. Callow, L. Coates, R. Dahint, R. Dalgliesh, N. A. Dencher, V. T. Forsyth, G. Fragneto, B. Frick, R. Gilles, T. Gutberlet, M. Haertlein, T. Hauss, W. Haussler, W. T. Heller, K. Herwig, O. Holderer, F. Juranyi, R. Kampmann, R. Knott, S. Krueger, P. Langan, R. E. Lechner, G. Lynn, C. Majkrzak, R. P. May, F. Meilleur, Y. Mo, K. Mortensen, D. A. A. Myles, F. Natali, C. Neylon, N. Niimura, J. Ollivier, A. Ostermann, J. Peters, J. Pieper, A. Ruhm, D. Schwahn, K. Shibata, A. K. Soper, T. Strassle, J. Suzuki, I. Tanaka, M. Tehei, P. Timmins, N. Torikai, T. Unruh, V. Urban, R. Vavrin, and K. Weiss, New sources and instrumentation for neutrons in biology, Chem. Phys., 345(2-3), 133-151 (2008).

69. J. Thorogood, B. J. Kennedy, M. Avdeev, and T. Kamiyama, The stability of Na-doped $Bi_2(NbCr)O_{7-x}$ pyrochlores: The non-existence of "$(BiNa)(NbCr)O_6$", J. Phys. Chem. Solids, 69(4), 918-922 (2008).

70. J. Thorogood, P. J. Saines, B. J. Kennedy, R. L. Withers, and M. M. Elcombe, Diffuse scattering in the cesium pyrochlore $CsTi_{0.5}W_{1.5}O_6$, Mater. Res. Bull., 43(4), 787-795 (2008).

71. C. Ton-That, M. R. Phillips, M. Foley, S. J. Moody, and A. P. J. Stampfl, Surface electronic properties of ZnO nanoparticles, Appl. Phys. Lett., 92(26), 3 (2008).

72. Trewhella, The different views from small angles, Proc. Natl. Acad. Sci. U. S. A., 105(13), 4967-4968 (2008).

73. P. Veder, R. De Marco, G. Clarke, R. Chester, A. Nelson, K. Prince, E. Pretsch, and E. Bakkert, Elimination of undesirable water layers in solid-contact polymeric ion-selective electrodes, Anal. Chem., 80(17), 6731-6740 (2008).

74. V. V. Volkov, V. A. Lapuk, E. V. Shtykova, N. D. Stepina, K. A. Dembo, A. V. Sokolova, S. V. Amarantov, V. P. Timofeev, R. K. Ziganshin, and E. Y. Varlamova, Structural features of Fab fragments of rheumatoid factor IgM-RF in solution, Crystallogr. Rep., 53(3), 466-473 (2008).

75. L. Wang, S. J. Campbell, A. J. Studer, M. Avdeev, M. Hofmann, M. Hoelzel, and S. X. Dou, Magnetic structures and phase transitions in $PrMn_{2-x}Fe_xGe_2$, J. Appl. Phys., 104(10), Art. No. 103911 (2008).

76. J. Walock, H. Ambaye, M. Chshiev, F. R. Klose, W. H. Butler, and G. J. Mankey, High magnetization FeCo/Pd multilayers, J. Vac. Sci. Technol. A, 26(4), 731-734 (2008).

77. A. S. Webster, C. D. Ling, C. L. Raston, and F. J. Lincoln, The structural and conductivity evolution of fluorite-type Bi_2O_3-Er_2O_3-PbO solid electrolytes during long-term annealing, Solid State Ion., 179(19-20), 697-705 (2008).

78. A. E. Whitten, S. Z. Ca, and J. Trewhella, MULCh: modules for the analysis of small-angle neutron contrast variation data from biomolecular assemblies, J. Appl. Crystallogr., 41, 222-226 (2008).

79. A. E. Whitten, C. M. Jeffries, S. P. Harris, and J. Trewhella, Cardiac myosin-binding protein C decorates F-actin: Implications for cardiac function, Proc. Natl. Acad. Sci. U. S. A., 105(47), 18360-18365 (2008).

80. Y. Wu, A. Kobayashi, G. J. Halder, V. K. Peterson, K. W. Chapman, N. Lock, P. D. Southon, and C. J. Kepert, Negative Thermal Expansion in the Metal-Organic Framework Material Cu_3(1,3,5-benzenetricarboxylate)$_2$, Angew. Chem.-Int. Edit., 47(46), 8929-8932 (2008)

81. E. J. Wolfson, E. N. Caspi, H. Ettedgui, H. Shaked, and M. Avdeev, Magnetic and crystallographic study of $Tb_{0.75}Y_{0.25}Co_3B_2$, J. Magn. Magn. Mater., 320(13), L97-L101 (2008).

82. C. Yang, C. M. Wu, W. H. Li, T. S. Chan, R. S. Liu, Y. Y. Chen, and M. Avdeev, Effects of oxygen deficiency on the magnetic ordering of Mn in $(TbNa_{0.1}MnO_{2.9})$-$Na_{0.9}$, J. Phys.-Condes. Matter, 20(10), Art. No. 104234 (2008).

83. S. I. Yun, D. Attard, V. Lo, J. Davis, H. Li, B. Latella, F. Tsvetkov, H. Noorman, S. Moricca, R. Knott, H. Hanley, M. Morcom, G. P. Simon, and G. E. Gadd, Spray-dried microspheres as a route to clay/polymer nanocomposites, J. Appl. Polym. Sci., 108(3), 1550-1556 (2008).

84. H. L. Zhan, M. Taraban, J. Trewhella, and L. Swint-Kruse, Subdividing repressor function: DNA binding affinity, selectivity, and allostery can be altered by amino acid substitution of nonconserved residues in a LacI/GalR homologue, Biochemistry, 47(31), 8058-8069 (2008).

2009

1. L. M. Anovitz, G. W. Lynn, D. R. Cole, G. Rother, L. F. Allard, W. A. Hamilton, L. Porcar, and M. H. Kim, A new approach to quantification of metamorphism using ultra-small and small angle neutron scattering, Geochim. Cosmochim. Acta 73, 7303-7324 (2009).

2. T. Baikie, G. M. H. Ng, S. Madhavi, S. S. Pramana, K. Blake, M. Elcombe, and T. J. White, The crystal chemistry of the alkaline-earth apatites $A_{10}(PO_4)_6Cu_xO_yH_z$ (A = Ca, Sr and Ba), Dalton Trans. 34, 6722-6726 (2009).

3. J. Blazek, and L. Copeland, Effect of monopalmitin on pasting properties of wheat starches with varying arnylose content, Carbohydr. Polym. 78, 131-136 (2009).

4. J. Blazek, H. Salman, A. L. Rubio, E. Gilbert, T. Hanley, and L. Copeland, Structural characterization of wheat starch granules differing in amylose content and functional characteristics, Carbohydr. Polym. 75, 705-711 (2009).

5. M. Bleuel, J. M. Carpenter, B. J. Micklich, P. Geltenbort, K. Mishima, H. M. Shimizu, Y. Iwashita, K. Hirota, M. Hino, S. J. Kennedy, and J. Lal, A small angle neutron scattering (SANS) experiment using very cold neutrons (VCN), Physica B 404, 2629-2632 (2009).

6. C. M. Brown, Y. Liu, T. Yildirim, V. K. Peterson, and C. J. Kepert, Hydrogen adsorption in HKUST-1: a combined inelastic neutron scattering and first-principles study, Nanotechnology 20, Art. No. 204025 (2009).

7. H. Cavaye, A. R. G. Smith, M. James, A. Nelson, P. L. Burn, I. R. Gentle, S. C. Lo, and P. Meredith, Solid-State Dendrimer Sensors: Probing the Diffusion of an Explosive Analogue Using Neutron Reflectometry, Langmuir 25, 12800-12805 (2009).

8. T. C. Chilcott, E. L. S. Wong, H. G. L. Coster, A. C. F. Coster, and M. James, Ionic double layer of atomically flat gold formed on mica templates, Electrochim. Acta 54, 3766-3774 (2009).

9. M. Choucair, P. Thordarson, and J. A. Stride, Gram-scale production of graphene based on solvothermal synthesis and sonication, Nat. Nanotechnol. 4, 30-33 (2009).

10. S. Ciampi, P. K. Eggers, G. Le Saux, M. James, J. B. Harper, and J. J. Gooding, Silicon (100) Electrodes Resistant to Oxidation in Aqueous Solutions: An Unexpected Benefit of Surface Acetylene Moieties, Langmuir 25, 2530-2539 (2009).

11. J. K. Claridge, S. J. Headey, J. Y. H. Chow, M. Schwalbe, P. J. Edwards, C. M. Jeffries, H. Venugopal, J. Trewhella, and S. M. Pascal, A picornaviral loop-to-loop replication complex, J. Struct. Biol. 166, 251-262 (2009).

12. L. Copeland, J. Blazek, H. Salman, and M. C. M. Tang, Form and functionality of starch, Food Hydrocolloids 23, 1527-1534 (2009).

13. K. E. Crompton, J. S. Forsythe, M. K. Horne, D. I. Finkelstein, and R. B. Knott, Molecular level and microstructural characterisation of thermally sensitive chitosan hydrogels, Soft Matter 5, 4704-4711 (2009).

14. S. A. Danilkin, An investigation of the structural dynamics in the fast ionic conductor $Cu_{2-\delta}Se$ using neutron scattering, J. Alloy. Compd. 467, 509-513 (2009).

15. S. A. Danilkin, Diffuse scattering and lattice dynamics of superionic copper chalcogenides, Solid State Ion. 180, 483-487 (2009).

16. A. V. Druker, C. Sobrero, J. Malarria, U. Garbe, H. G. Brokmeier, and R. E. Bolmaro, Effect of texture heterogeneities on the shape memory properties of rolled Fe-Mn-Si SMA, Z. Kristallogr. Suppl. 30, 297-302 (2009).

17. W. K. Fong, T. Hanley, and B. J. Boyd, Stimuli responsive liquid crystals provide 'on-demand' drug delivery in vitro and in vivo, J. Control. Release 135, 218-226 (2009).

18. F. Fontaine-Vive, F. Merzel, M. R. Johnson, and G. J. Kearley, Collagen and component polypeptides: Low frequency and amide vibrations, Chem. Phys. 355, 141-148 (2009).

19. U. Garbe, New pole figure calculation software: 2DiffCalc, J. Appl. Crystallogr. 42, 730-733 (2009).

20. A. Ghahghaei, A. Rekas, J. A. Carver, and R. C. Augusteyn, Structure/function studies of dogfish alpha-crystallin, comparison with bovine alpha-crystallin, Mol. Vis. 15, 2411-2420 (2009).

21. R. Giulian, L. L. Araujo, P. Kluth, D. J. Sprouster, C. S. Schnohr, G. J. Foran, and M. C. Ridgway, Temperature-dependent EXAFS analysis of embedded Pt nanocrystals, J. Phys.-Condes. Matter 21, Art. No. 155302 (2009).

22. R. Giulian, L. L. Araujo, P. Kluth, D. J. Sprouster, C. S. Schnohr, B. Johannessen, G. J. Foran, and M. C. Ridgway, The influence of annealing conditions on the growth and structure of embedded Pt nanocrystals, J. Appl. Phys. 105, Art. No. 044303 (2009).

23. D. J. Goossens, A. G. Beasley, T. R. Welberry, M. J. Gutmann, and R. O. Piltz, Neutron diffuse scattering in deuterated para-terphenyl, $C_{18}D_{14}$, J. Phys.-Condes. Matter 21, Art. No. 124204 (2009).

24. A. Htoon, A. K. Shrestha, B. M. Flanagan, A. Lopez-Rubio, A. R. Bird, E. P. Gilbert, and M. J. Gidley, Effects of processing high amylose maize starches under controlled conditions on structural organisation and amylase digestibility, Carbohydr. Polym. 75, 236-245 (2009).

25. J. M. Hudspeth, D. J. Goossens, A. J. Studer, R. L. Withers, and L. Noren, The crystal and magnetic structures of $LaCa_2Fe_3O_8$ and $NdCa_2Fe_3O_8$, J. Phys.-Condes. Matter 21, Art. No. 124206 (2009).

26. D. A. Jacques, M. Streamer, S. L. Rowland, G. F. King, J. M. Guss, J. Trewhella, and D. B. Langley, Structure of the sporulation histidine kinase inhibitor Sda from Bacillus subtilis and insights into its solution state, Acta Crystallogr. Sect. D-Biol. Crystallogr. 65, 574-581 (2009).

27. P. C. Ju, G. Pages, R. P. Riek, P. C. Chen, A. M. Torres, P. S. Bansal, S. Kuyucak, P. W. Kuchel, and J. I. Vandenberg, The Pore Domain Outer Helix Contributes to Both Activation and Inactivation of the hERG K+ Channel, J. Biol. Chem. 284, 1000-1008 (2009).

28. N. Kamarulzaman, R. Yusoff, N. Kamarudin, N. H. Shaari, N. A. A. Aziz, M. A. Bustam, N. Blagojevic, M. Elcombe, M. Blackford, M. Avdeev, and A. K. Arof, Investigation of cell parameters, microstructures and electrochemical behaviour of $LiMn_2O_4$ normal and nano powders, J. Power Sources 188, 274-280 (2009).

29. B. Kent, C. J. Garvey, D. Cookson, and G. Bryant, The inverse hexagonal - inverse ribbon - lamellar gel phase transition sequence in low hydration DOPC:DOPE phospholipid mixtures, Chem. Phys. Lipids 157, 56-60 (2009).

30. O. Kirstein, M. Prager, and G. J. Schneider, Rotational dynamics and coupling of methyl group rotations in methyl fluoride studied by high resolution inelastic neutron scattering, J. Chem. Phys. 130, Art. No. 214508 (2009).

31. J. M. S. Koh, P. S. Bansal, A. M. Torres, and P. W. Kuchel, PLATYPUS venom: source of novel compounds, Aust. J. Zool. 57, 203-210 (2009).

32. Y. Lauw, M. D. Horne, T. Rodopoulos, N. A. S. Webster, B. Minofar, and A. Nelson, X-Ray reflectometry studies on the effect of water on the surface structure of [C4mpyr][NTf_2] ionic liquid, Phys. Chem. Chem. Phys. 11, 11507-11514 (2009).

33. B. M. Law, M. D. Brown, L. Marchand, L. B. Lurio, W. A. Hamilton, I. Kuzmenko, T. Gog, S. Satija, E. Watkins, and J. Majewski, Adsorption at liquid interfaces: A comparison of multiple experimental techniques, Eur. Phys. J.-Spec. Top. 167, 127-132 (2009).

34. A. Le Bail, L. M. D. Cranswick, K. Adil, A. Altomare, M. Avdeev, R. Cerny, C. Cuocci, C. Giacovazzo, I. Halasz, S. H. Lapidus, J. N. Louwen, A. Moliterni, L. Palatinus, R. Rizzi, E. C. Schilder, P. W. Stephens, K. H. Stone, and J. van Mechelen, Third structure determination by powder diffractometry round robin (SDPDRR-3), Powder Diffr. 24, 254-262 (2009).

35. B. Lee, H. Wacklin, and C. D. Bain, Changes in molecular composition and packing during lipid membrane reconstitution from phospholipid-surfactant micelles, Soft Matter 5, 568-575 (2009).

36. K. W. Y. Lee, T. H. Nguyen, T. Hanley, and B. J. Boyd, Nanostructure of liquid crystalline matrix determines in vitro sustained release and in vivo oral absorption kinetics for hydrophilic model drugs, Int. J. Pharm. 365, 190-199 (2009).

37. T. Lenne, C. J. Garvey, K. L. Koster, and G. Bryant, Effects of Sugars on Lipid Bilayers during Dehydration - SAXS/WAXS Measurements and Quantitative Model, J. Phys. Chem. B 113, 2486-2491 (2009).

38. C. D. Ling, M. Avdeev, R. Kutteh, V. V. Kharton, A. A. Yaremchenko, S. Fialkova, N. Sharma, R. B. Macquart, M. Hoelzel, and M. Gutmann, Structures, Phase Transitions, Hydration, and Ionic Conductivity of $Ba_4Nb_2O_9$, Chem. Mat. 21, 3853-3864 (2009).

39. C. D. Ling, B. Rowda, M. Avdeev, and R. Pullar, Structures, phase transitions and microwave dielectric properties of the 6H perovskites $Ba_3BSb_2O_9$, B = Mg, Ca, Sr, Ba, J. Solid State Chem. 182, 479-483 (2009).

40. K. D. Liss, T. d'Almeida, M. Kaiser, R. Hock, A. Magerl, and J. F. Eloy, Time-resolved x-ray diffraction study of laser-induced shock and acoustic waves in single crystalline silicon, J. Appl. Phys. 106, Art. No. 044914 (2009).

41. K. D. Liss, U. Garbe, H. J. Li, T. Schambron, J. D. Almer, and K. Yan, In Situ Observation of Dynamic Recrystallization in the Bulk of Zirconium Alloy, Adv. Eng. Mater. 11, 637-640 (2009).

42. K. D. Liss, R. E. Whitfield, W. Xu, T. Buslaps, L. A. Yeoh, X. L. Wu, D. L. Zhang, and K. N. Xia, In situ synchrotron high-energy X-ray diffraction analysis on phase transformations in Ti-Al alloys processed by equal-channel angular pressing, J. Synchrot. Radiat. 16, 825-834 (2009).

43. K. D. Liss, T. Schmoelzer, K. Yan, M. Reid, M. Peel, R. Dippenaar, and H. Clemens, In situ study of dynamic recrystallization and hot deformation behavior of a multiphase titanium aluminide alloy, J. Appl. Phys. 106, Art. No. 113526 (2009).

44. A. Lopez-Rubio, J. M. Clarke, B. Scherer, D. L. Topping, and E. P. Gilbert, Structural modifications of granular starch upon acylation with short-chain fatty acids, Food Hydrocolloids 23, 1940-1946 (2009).

45. A. Lopez-Rubio, and E. P. Gilbert, Neutron scattering: a natural tool for food science and technology research, Trends Food Sci. Technol. 20, 576-586 (2009).

46. Z. Lu, M. J. Walock, P. R. LeClair, G. J. Mankey, P. Mani, D. Lott, F. Klose, H. Ambaye, V. Lauter, M. Wolff, A. Schreyer, H. M. Christen, and B. C. Sales, Structural and magnetic properties of epitaxial $Fe_{25}Pt_{75}$, J. Vac. Sci. Technol. A 27, 770-775 (2009).

47. V. Luca, G. Soler-Illia, P. C. Angelome, P. Y. Steinberg, E. Drabarek, and T. L. Hanley, Striving for order and compositional homogeneity in bulk mesoporous zirconium titanium mixed metal oxides from triblock copolymers and metal chlorides, Microporous Mesoporous Mat. 118, 443-452 (2009).

48. L. A. Meure, R. Knott, N. R. Foster, and F. Dehghani, The Depressurization of an Expanded Solution into Aqueous Media for the Bulk Production of Liposomes, Langmuir 25, 326-337 (2009).

49. R. D. Mills, J. Trewhella, T. W. Qiu, T. Welte, T. M. Ryan, T. Hanley, R. B. Knott, T. Lithgow, and T. D. Mulhern, Domain Organization of the Monomeric Form of the Tom70 Mitochondrial Import Receptor, J. Mol. Biol. 388, 1043-1058 (2009).

50. A. M. Mulders, S. M. Lawrence, U. Staub, M. Garcia-Fernandez, V. Scagnoli, C. Mazzoli, E. Pomjakushina, K. Conder, and Y. Wang, Direct Observation of Charge Order and an Orbital Glass State in Multiferroic $LuFe_2O_4$, Phys. Rev. Lett. 103, Art. No. 077602 (2009).

51. A. M. Mulders, H. Loosvelt, A. F. Rodriguez, E. Popova, T. Konishi, K. Temst, O. Karis, D. Arvanitis, and C. Van Haesendonck, On the interface magnetism of thin oxidized Co films: orbital and spin moments, J. Phys.-Condes. Matter 21, Art. No. 124211 (2009).

52. Y. Mulyana, A. Nafady, A. Mukherjee, R. Bircher, B. Moubaraki, K. S. Murray, A. M. Bond, B. F. Abrahams, and C. Boskovic, New Family of Ferric Spin Clusters Incorporating Redox-Active ortho-Dioxolene Ligands, Inorg. Chem. 48, 7765-7781 (2009).

53. Neto, M. James, and A. M. Telford, On the Composition of the Top Layer of Microphase Separated Thin PS-PEO Films, Macromolecules 42, 4801-4808 (2009).

54. M. C. C. Ng, D. J. Craig, J. B. Harper, L. Van-Eijck, and J. A. Stride, The Central Atom Size Effect on the Structure of Group 14 Tetratolyls, Chem.-Eur. J. 15, 6569-6572 (2009).

55. A. Ng, S. Ciampi, M. James, J. B. Harper, and J. J. Gooding, Comparing the Reactivity of Alkynes and Alkenes on Silicon (100) Surfaces, Langmuir 25, 13934-13941 (2009).

56. L. Noren, R. L. Withers, D. J. Goossens, M. Elcombe, and G. J. Kearley, Coupled Li^{1+}/Nb^{5+} and O^{2-}/F^{-} ordering on the Na and Cl sites of the average NaCl structure of Li_4NbO_4F, J. Solid State Chem. 182, 1109-1114 (2009).

57. G. Pages, A. M. Torres, P. C. Ju, P. S. Bansal, P. F. Alewood, P. W. Kuchel, and J. I. Vandenberg, Structure of the pore-helix of the hERG K+ channel, Eur. Biophys. J. Biophys. Lett. 39, 111-120 (2009).

58. V. K. Peterson, and A. E. Whitten, Hydration Processes in Tricalcium Silicate: Application of the Boundary Nucleation Model to Quasielastic Neutron Scattering Data, J. Phys. Chem. C, 113(6), 2347-2351 (2009).

59. M. Pooke, V. Chamritski, M. Fee, S. Gibson, B. T. King, J. L. Tallon, M. Meissner, R. Feyerherm, S. R. Olsen, S. J. Kennedy, and R. A. Robinson, HTS 5 Tesla Synchrotron and Neutron Beamline Magnets, IEEE Trans. Appl. Supercond. 19, 1372-1375 (2009).

60. A. Rekas, V. Lo, G. E. Gadd, R. Cappai, and S. L. Yun, PAMAM Dendrimers as Potential Agents against Fibrillation of alpha-Synuclein, a Parkinson's Disease-Related Protein, Macromol. Biosci. 9, 230-238 (2009).

61. M. Rahlenbeck, G. L. Sun, D. L. Sun, C. T. Lin, B. Keimer, and C. Ulrich, Phonon anomalies in pure and underdoped $R_{1-x}K_xFe_2As_2$ (R = Ba, Sr) investigated by Raman light scattering, Phys. Rev. B 80, Art. No. 064509 (2009).

62. P. A. Reynolds, E. P. Gilbert, M. J. Henderson, and J. W. White, Structure of High Internal Phase Aqueous-in-Oil Emulsions and Related Inverse Micelle Solutions. 3. Variation of Surfactant, J. Phys. Chem. B 113, 12231-12242 (2009).

63. P. A. Reynolds, E. P. Gilbert, M. J. Henderson, and J. W. White, Structure of High Internal Phase Aqueous-in-Oil Emulsions and Related Inverse Micelle Solutions. 4. Surfactant Mixtures, J. Phys. Chem. B 113, 12243-12256 (2009).

64. M. C. Ridgway, P. Kluth, R. Giulian, D. J. Sprouster, L. L. Araujo, C. S. Schnohr, D. J. Llewellyn, A. P. Byrne, G. J. Foran, and D. J. Cookson, Changes in metal nanoparticle shape and size induced by swift heavy-ion irradiation, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms 267, 931-935 (2009).

65. S. B. Rizwan, T. Hanley, B. J. Boyd, T. Rades, and S. Hook, Liquid Crystalline Systems of Phytantriol and Glyceryl Monooleate Containing a Hydrophilic Protein: Characterisation, Swelling and Release Kinetics, J. Pharm. Sci. 98, 4191-4204 (2009).

66. H. Salman, J. Blazek, A. Lopez-Rubio, E. P. Gilbert, T. Hanley, and L. Copeland, Structure-function relationships in A and B granules from wheat starches of similar amylose content, Carbohydr. Polym. 75, 420-427 (2009).

67. S. Schnohr, P. Kluth, L. L. Araujo, D. J. Sprouster, A. P. Byrne, G. J. Foran, and M. C. Ridgway, Anisotropic vibrations in crystalline and amorphous InP, Phys. Rev. B, 79, Art. No. 195203 (2009).

68. N. Sharma, R. B. Macquart, M. Christensen, M. Avdeev, Y. S. Chen, and C. D. Ling, Structure and crystal chemistry of fluorite-related $Bi_{38}Mo_7O_{78}$ from single crystal X-ray diffraction and ab initio calculations, J. Solid State Chem. 182, 1312-1318 (2009).

69. N. Sharma, R. L. Withers, K. S. Knight, and C. D. Ling, Structure, crystal chemistry and thermal evolution of the delta-Bi_2O_3-related phase Bi_9ReO_{17}, J. Solid State Chem., 182(9), 2468-2474 (2009).

70. K. S. Siddiqui, D. M. Parkin, P. M. G. Curmi, D. De Francisci, A. Poljak, K. Barrow, M. H. Noble, J. Trewhella, and R. Cavicchioli, A Novel Approach for Enhancing the Catalytic Efficiency of a Protease at Low Temperature: Reduction in Substrate Inhibition by Chemical Modification, Biotechnol. Bioeng. 103, 676-686 (2009).

71. J. Sprouster, R. Giulian, C. S. Schnohr, L. L. Araujo, P. Kluth, A. P. Byrne, G. J. Foran, B. Johannessen, and M. C. Ridgway, fcc-hcp phase transformation in Co nanoparticles induced by swift heavy-ion irradiation, Phys. Rev. B, 80, Art. No. 115438 (2009).

72. W. Sriprom, M. James, S. Perrier, and C. Neto, Ordered Microphase Separation in Thin Films of PMMA-PBA Synthesized by RAFT: Effect of Block Polydispersity, Macromolecules 42, 3138-3146 (2009).

73. Y. J. Sun, D. D. Qu, Y. J. Huang, K. D. Liss, X. S. Wei, D. W. Xing, and J. Shen, Zr-Cu-Ni-Al bulk metallic glasses with superhigh glass-forming ability, Acta Mater. 57, 1290-1299 (2009).

74. D. Szekely, T. Yau, and P. Kuchel, Human erythrocyte flickering: temperature, ATP concentration, water transport, and cell aging, plus a computer simulation, Eur. Biophys. J. 38, 923-939 (2009).

75. J. Thorogood, B. J. Kennedy, V. K. Peterson, M. M. Elcombe, G. J. Kearley, J. V. Hanna, and V. Luca, Anomalous lattice parameter increase in alkali earth aluminium substituted tungsten defect pyrochlores, J. Solid State Chem. 182, 457-464 (2009).

76. J. Ting, B. J. Kennedy, R. L. Withers, and M. Avdeev, Synthesis and structural studies of lanthanide substituted bismuth-titanium pyrochlores, J. Solid State Chem. 182, 836-840 (2009).

77. E. V. Tsipis, J. C. Waerenborgh, M. Avdeev, and V. V. Kharton, Mossbauer spectroscopy analysis of Fe-57-doped $YBaCo_4O_{7+delta}$: Effects of oxygen intercalation, J. Solid State Chem. 182, 640-643 (2009).

78. L. van Eijck, A. S. Best, S. Long, F. Fernandez-Alonso, D. MacFarlane, M. Forsyth, and G. J. Kearley, Localized Relaxational Dynamics of Succinonitrile, J. Phys. Chem. C 113, 15007-15013 (2009).

79. H. P. Wacklin, Interfacial Mechanism of Phospholipase A2: pH-Dependent Inhibition and Me-Î²-cyclodextrin Activation, Biochemistry 48, 5874-5881 (2009).

80. J. L. Wang, S. J. Campbell, A. J. Studer, M. Avdeev, R. Zeng, and S. X. Dou, Magnetic phase transitions in $Pr_{1-x}Lu_xMn_2Ge_2$ compounds, J. Phys.-Condes. Matter 21, Art. No. 124217 (2009).

81. J. L. Wang, S. J. Campbell, R. Zeng, C. K. Poh, S. X. Dou, and S. J. Kennedy, Re-entrant ferromagnet PrMn2Ge0.8Si1.2: Magnetocaloric effect, J. Appl. Phys. 105, Art. No. 07A909 (2009).

82. Y. M. Wang, P. Wang, D. Kohls, W. A. Hamilton, and D. W. Schaefer, Water absorption and transport in bis-silane films, Phys. Chem. Chem. Phys. 11, 161-166 (2009).

83. I. J. Watson, K. D. Liss, H. Clemens, W. Wallgram, T. Schmoelzer, T. C. Hansen, and M. Reid, In Situ Characterization of a Nb and Mo Containing gamma-TiAl Based Alloy Using Neutron Diffraction and High-Temperature Microscopy, Adv. Eng. Mater. 11, 932-937 (2009).

84. C. E. White, J. L. Provis, D. P. Riley, G. J. Kearley, and J. S. J. van Deventer, What Is the Structure of Kaolinite? Reconciling Theory and Experiment, J. Phys. Chem. B 113, 6756-6765 (2009).

85. A. E. Whitten, B. J. Smith, J. G. Menting, M. B. Margetts, N. M. McKern, G. O. Lovrecz, T. E. Adams, K. Richards, J. D. Bentley, J. Trewhella, C. W. Ward, and M. C. Lawrence, Solution Structure of Ectodomains of the Insulin Receptor Family: The Ectodomain of the Type 1 Insulin-Like Growth Factor Receptor Displays Asymmetry of Ligand Binding Accompanied by Limited Conformational Change, J. Mol. Biol., 394, 878-892 (2009).

86. S. Yakovlev, M. Avdeev, and M. Mezouar, High-pressure structural behavior and equation of state of $NaZnF_3$, J. Solid State Chem. 182, 1545-1549 (2009).

87. K. Yan, K.-D. Liss, U. Garbe, J. Daniels, O. Kirstein, H. Li, and R. Dippenaar, From Single Grains to Texture, Adv. Eng. Mater. 11, 771-773 (2009).

88. D. H. Yu, J. Duriavig, N. Loh, R. Woodward, H. J. Lin, F. H. Chang, S. H. Kilcoyne, A. Stampfl, and R. A. Robinson, Investigation of field-induced ferromagnetism in Pd-Ni-Fe-P metallic glass by x-ray magnetic circular dichroism, Appl. Phys. Lett. 94, Art. No. 022502 (2009).

89. J. Yu, D. H. Yu, Y. Chen, H. Chen, M. Y. Lin, B. M. Cheng, J. Li, and W. H. Duan, Narrowed bandgaps and stronger excitonic effects from small boron nitride nanotubes, Chem. Phys. Lett. 476, 240-243 (2009).

90. Q. D. Zhou, B. J. Kennedy, M. Avdeev, L. Giachini, and J. A. Kimpton, Structural studies of the phases in Ba_2LaIrO_6-New light on an old problem, J. Solid State Chem. 182, 3195-3200 (2009).

2010

1. L. Arai, M. A. Nadeem, M. Bhadbhade, and J. A. Stride, A 2D cobalt based coordination polymer constructed from benzimidazole and acetate ion exhibiting spin-canted antiferromagnetism, Dalton Trans., 39(14), 3372-3374 (2010).

2. M. Avdeev, V. V. Kharton, and E. V. Tsipis, Geometric parameterization of the $YBaCo_4O_7$ structure type: Implications for stability of the hexagonal form and oxygen uptake, J. Solid State Chem., 183(10), 2506-2509 (2010).

3. J. E. Bateman, R. M. Dalgleish, D. M. Duxbury, S. A. Holt, D. J. McPhail, A. S. Marsh, N. J. Rhodes, E. M. Schooneveld, E. J. Spill and R. Stephenson, The FastGas Detetector, Nucl. Instrum. Meth. A 616, 59-64 (2010).

4. J. L. P. Benesch, J. A. Aquilina, A. J. Baldwin, A. Rekas, F. Stengel, R. A. Lindner, E. Basha, G. L. Devlin, J. Horwitz, E. Vierling, J. A. Carver, and C. V. Robinson, The Quaternary Organization and Dynamics of the Molecular Chaperone HSP26 Are Thermally Regulated, Chem. Biol., 17(9), 1008-1017 (2010).

5. G. Berecki, L. Motin, A. Haythornthwaite, S. Vink, P. Bansal, R. Drinkwater, C. I. Wang, M. Moretta, R. J. Lewis, P. F. Alewood, M. J. Christie, and D. J. Adams, Analgesic omega-Conotoxins CVIE and CVIF Selectively and Voltage-Dependently Block Recombinant and Native N-Type Calcium Channels, Mol. Pharmacol., 77(2), 139-148 (2010).

6. J. Blazek, and L. Copeland, Amylolysis of wheat starches. I. Digestion kinetics of starches with varying functional properties, J. Cereal Sci., 51(3), 265-270 (2010).

7. J. Blazek, and L. Copeland, Amylolysis of wheat starches. II. Degradation patterns of native starch granules with varying functional properties, J. Cereal Sci., 52(2), 295-302 (2010).

8. M. P. Boland, C. R. Hatty, F. Separovic, A. F. Hill, D. J. Tew, K. J. Barnham, C. L. Haigh, M. James, C. L. Masters, and S. J. Collins, Anionic Phospholipid Interactions of the Prion Protein N Terminus Are Minimally Perturbing and Not Driven Solely by the Octapeptide Repeat Domain, J. Biol. Chem., 285(42), 32282-32292 (2010).

9. S. J. Bonyhady, C. Jones, S. Nembenna, A. Stasch, A. J. Edwards, and G. J. McIntyre, beta-Diketiminate-Stabilized Magnesium(I) Dimers and Magnesium(II) Hydride Complexes: Synthesis, Characterization, Adduct Formation, and Reactivity Studies, Chem.-Eur. J., 16(3), 938-955 (2010).

10. P. Boyd, A. Edwards, M. Gardiner, C. Ho, M. H. Lemée-Cailleau, D. McGuinness, A. Riapanitra, J. Steed, D. Stringer, and B. Yates, Reduction of a Chelating Bis(NHC) Palladium(II) Complex to $[\{\mu\text{-bis(NHC)}\}_2Pd_2H]^+$: A Terminal Hydride in a Binuclear Palladium(I) Species Formed under Catalytically Relevant Conditions, Angew. Chem.-Int. Edit., 49(36), 6315-6318 (2010).

11. W. R. Brant, S. Schmid, Q. F. Gu, R. L. Withers, J. Hester, and M. Avdeev, Temperature and composition dependent structural investigation of the defect perovskite series $Sr_{1-x}Ti_{1-2x}Nb_{2x}O_3$, 0 <= x <= 0.2, J. Solid State Chem., 183(9), 1998-2003 (2010).

12. B. L. Caba, Q. Zhang, M. R. J. Carroll, R. C. Woodward, T. G. St Pierre, E. P. Gilbert, J. S. Riffle, and R. M. Davis, Nanostructure of PEO-polyurethane-PEO triblock copolymer micelles in water, J. Colloid Interface Sci., 344(1), 81-89 (2010).

13. M. R. J. Carroll, R. C. Woodward, M. J. House, W. Y. Teoh, R. Amal, T. L. Hanley, and T. G. St Pierre, Experimental validation of proton transverse relaxivity models for superparamagnetic nanoparticle MRI contrast agents, Nanotechnology, 21(3), Art. No. 035103 (2010).

14. S. L. Chou, J. Z. Wang, M. Choucair, H. K. Liu, J. A. Stride, and S. X. Dou, Enhanced reversible lithium storage in a nanosize silicon/graphene composite, Electrochem. Commun., 12(2), 303-306 (2010).

15. J. Y. H. Chow, C. M. Jeffries, A. H. Kwan, J. M. Guss, and J. Trewhella, Calmodulin Disrupts the Structure of the HIV-1 MA Protein, J. Mol. Biol., 400(4), 702-714 (2010).

16. D. Comoletti, M. T. Miller, C. M. Jeffries, J. Wilson, B. Demeler, P. Taylor, J. Trewhella, and T. Nakagawa, The Macromolecular Architecture of Extracellular Domain of alpha NRXN1: Domain Organization, Flexibility, and Insights into Trans-Synaptic Disposition, Structure, 18(8), 1044-1053 (2010).

17. A. J. Cross, C. M. Jeffries, J. Trewhella, and J. M. Matthews, LIM Domain Binding Proteins 1 and 2 Have Different Oligomeric States, J. Mol. Biol., 399(1), 133-144 (2010).

18. S. A. Danilkin, M. Yethiraj, and G. J. Kearley, Phonon Dispersion in Superionic Copper Selenide: Observation of Soft Phonon Modes in Superionic Phase Transition, J. Phys. Soc. Jpn., 79, Supplement A, 25-28 (2010).

19. T. A. Darwish, R. A. Evans, M. James, N. Malic, G. Triani, and T. L. Hanley, CO_2 Triggering and Controlling Orthogonally Multiresponsive Photochromic Systems, J. Am. Chem. Soc., 132(31), 10748-10755 (2010).

20. Y. D. Dong, A. J. Tilley, I. Larson, M. J. Lawrence, H. Amenitsch, M. Rappolt, T. Hanley, and B. J. Boyd, Nonequilibrium Effects in Self-Assembled Mesophase Materials: Unexpected Supercooling Effects for Cubosomes and Hexosomes, Langmuir, 26(11), 9000-9010 (2010).

21. A. W. Fenton, R. Williams, and J. Trewhella, Changes in Small-Angle X-ray Scattering Parameters Observed upon Binding of Ligand to Rabbit Muscle Pyruvate Kinase Are Not Correlated with Allosteric Transitions, Biochemistry, 49(33), 7202-7209 (2010).

22. W. K. Fong, T. L. Hanley, B. Thierry, N. Kirby, and B. J. Boyd, Plasmonic Nanorods Provide Reversible Control over Nanostructure of Self-Assembled Drug Delivery Materials, Langmuir, 26(9), 6136-6139 (2010).

23. Y. Gao, A. Heinemann, R. Knott, and J. Bartlett, Encapsulation of Protein in Silica Matrices: Structural Evolution on the Molecular and Nanoscales, Langmuir, 26(2), 1239-1246 (2010).

24. D. J. Goossens, A. J. Studer, and Z. H. Stachurski, Microstructure of Horseshoe Nails Using Neutron Diffraction, J. Mater. Eng. Perform., 19(3), 380-384 (2010).

25. I. E. Grey, I. C. Madsen, S. J. Mills, F. Hatert, V. K. Peterson, and T. J. Bastow, A new type of cubic-stacked layer structure in anthoinite, $AlWO_3(OH)_3$, Am. Miner., 95(4), 639-645 (2010).

26. N. Hameed, Q. P. Guo, T. Hanley, and Y. W. Mai, Hydrogen Bonding Interactions, Crystallization, and Surface Hydrophobicity in Nanostructured Epoxy/Block Copolymer Blends, J. Polym. Sci. Pt. B-Polym. Phys., 48(7), 790-800 (2010).

27. A. K. Htoon, S. Uthayakumaran, U. Piyasiri, I. A. M. Appelqvist, A. López-Rubio, E. P. Gilbert, and R. J. Mulder, The effect of acid dextrinisation on enzyme-resistant starch content in extruded maize starch, Food Chem., 120(1), 140-149 (2010).

28. T. W. Huang, T. K. Chen, K. W. Yeh, C. T. Ke, C. L. Chen, Y. L. Huang, F. C. Hsu, M. K. Wu, P. M. Wu, M. Avdeev, and A. J. Studer, Doping-driven structural phase transition and loss of superconductivity in $M_xFe_{1-x}Se_{delta}$ (M=Mn, Cu), Phys. Rev. B, 82(10), Art. No. 104502 (2010).

29. D. A. Jacques, and J. Trewhella, Small-angle scattering for structural biology-Expanding the frontier while avoiding the pitfalls, Protein Sci., 19(4), 642-657 (2010).

30. M. James, M. L. Carter, Z. M. Zhang, Y. J. Zhang, K. S. Wallwork, M. Avdeev, and E. R. Vance, Crystal Chemistry and Structures of (Ca,U) Titanate Pyrochlores, J. Am. Ceram. Soc., 93(10), 3464-3473 (2010).

31. V. V. Kharton, M. V. Patrakeev, E. V. Tsipis, M. Avdeev, E. N. Naumovich, P. V. Anikina, and J. C. Waerenborgh, Oxygen nonstoichiometry, chemical expansion, mixed conductivity, and anodic behavior of Mo-substituted $Sr_3Fe_2O_{7-delta}$, Solid State Ion., 181(21-22), 1052-1063 (2010).

32. C. S. Kealley, A. V. Sokolova, G. J. Kearley, E. Kemner, M. Russina, A. Faraone, W. A. Hamilton, and E. P. Gilbert, Dynamical transition in a large globular protein: Macroscopic properties and glass transition, BBA-Proteins Proteomics, 1804, 34-40 (2010).

33. G. J. Kearley and M. R. Johnson, Vibrational Spectroscopy with Neutrons Where Are We Now?, J. Vibspec. 53, 54-59 (2010).

34. B. Kent, C. J. Garvey, T. Lenne, L. Porcar, V. M. Garamus, and G. Bryant, Measurement of glucose exclusion from the fully hydrated DOPE inverse hexagonal phase, Soft Matter, 6(6), 1197-1202 (2010).

35. S. A. J. Kimber, C. D. Ling, J. P. Morris, A. Chemseddine, P. F. Henry, and D. N. Argyriou, Interlayer tuning of electronic and magnetic properties in honeycomb ordered $Ag_3LiRu_2O_6$, J. Mater. Chem., 20(37), 8021-8025 (2010).

36. E. H. Kisi, J. F. Zhang, O. Kirstein, D. P. Riley, M. J. Styles, and A. M. Paradowska, Shear stiffness in nanolaminar Ti_3SiC_2 challenges ab initio calculations, J. Phys.-Condes. Matter, 22(16), Art. No. 162202 (2010).

37. R. B. Knott, International Conference on Neutrons in Biology, Acta Cryst. D 66,1124-1125 (2010).

38. X. J. Kuang, Y. D. Li, C. D. Ling, R. L. Withers, and I. R. Evans, Oxide Ion Conductivity, Phase Transitions, and Phase Separation in Fluorite-Based $Bi_{38-x}Mo_{7+x}O_{78+1.5x}$, Chem. Mat., 22(15), 4484-4494 (2010).

39. Y. Lauw, M. D. Horne, T. Rodopoulos, A. Nelson, and F. A. M. Leermakers, Electrical Double-Layer Capacitance in Room Temperature Ionic Liquids: Ion-Size and Specific Adsorption Effects, J. Phys. Chem. B, 114(34), 11149-11154 (2010).

40. Y. Lauw, T. Rodopoulos, M. Gross, A. Nelson, R. Gardner, and M. D. Horne, Electrochemical cell for neutron reflectometry studies of the structure of ionic liquids at electrified interface, Rev. Sci. Instrum., 81(7), Art. No. 074101 (2010).

41. T. Lenne, C. J. Garvey, K. L. Koster, and G. Bryant, Kinetics of the lamellar gel-fluid transition in phosphatidylcholine membranes in the presence of sugars, Chem. Phys. Lipids, 163(2), 236-242 (2010).

42. E. Levy, L. K. Chan, D. H. Yu, M. M. Koza, Y. Mastai, R. C. Ford, and J. C. Li, Neutron scattering study of water confined in periodic mesoporous organosilicas, J. Solid State Chem., 183(7), 1691-1696 (2010).

43. X. L. Li, K. F. Cai, H. Li, D. H. Yu, X. Wang, and H. F. Wang, Alumina template-assisted electrodeposition of $Bi_2Te_{2.7}Se_{0.3}$ nanowire arrays, Superlattices Microstruct., 47(6), 710-713 (2010).

44. C. D. Ling, M. Avdeev, V. V. Kharton, A. A. Yaremchenko, R. B. Macquart, and M. Hoelzel, Structures, Phase Transitions, Hydration, and Ionic Conductivity of $Ba_4Ta_2O_9$, Chem. Mat., 22(2), 532-540 (2010).

45. C. D. Ling, B. J. Kennedy, Q. D. Zhou, J. R. Spencer, and M. Avdeev, Synthesis, structures, and phase transitions of barium bismuth iridium oxide perovskites Ba_2BiIrO_6 and $Ba_3BiIr_2O_9$, J. Solid State Chem., 183(3), 727-735 (2010).

46. N. Lock, Y. Wu, M. Christensen, L. J. Cameron, V. K. Peterson, A. J. Bridgeman, C. J. Kepert, and B. B. Iversen, Elucidating Negative Thermal Expansion in MOF-5, J. Phys. Chem. C, 114(39), 16181-16186 (2010).

47. V. Luca, E. Drabarek, C. S. Griffith, and T. L. Hanley, Understanding the Supramolecular Self-Assembly of Zirconium Titanate Mesophases Formed from the Poly(ethylene oxide) Surfactant Brij-58, Chem. Mat., 22(13), 3832-3842 (2010).

48. R. B. Macquart, B. J. Kennedy, and M. Avdeev, A primitive tetragonal intermediate in the orthorhombic-cubic phase transition of perovskite-type strontium niobate $Sr_{0.92}NbO_3$, J. Solid State Chem., 183(10), 2400-2405 (2010).

49. R. B. Macquart, B. J. Kennedy, and M. Avdeev, Neutron diffraction study of phase transitions in perovskite-type strontium molybdate $SrMoO_3$, J. Solid State Chem., 183(1), 250-255 (2010).

50. M. K. Mistry, N. R. Choudhury, N. K. Dutta, and R. Knott, Inorganic modification of block copolymer for medium temperature proton exchange membrane application, J. Membr. Sci., 351(1-2), 168-177 (2010).

51. A. M. Mulders, S. M. Lawrence, A. J. Princep, U. Staub, Y. Bodenthin, M. Garcia-Fernandez, M. Garganourakis, J. Hester, R. Macquart, and C. D. Ling, Circularly polarized soft x-ray diffraction study of helical magnetism in hexaferrite, Phys. Rev. B, 81(9), Art. No. 092405 (2010).

52. O. Muransky, M. R. Barnett, V. Luzin, and S. Vogel, On the correlation between deformation twinning and Luders-like deformation in an extruded Mg alloy: In situ neutron diffraction and EPSC.4 modelling, Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process., 527(6), 1383-1394 (2010).

53. M. A. Nadeem, M. Bhadbhade, R. Bircher, and J. A. Stride, Three isolated structural motifs in one crystal: penetration of two 1D chains through large cavities within 2D polymeric sheets, Crystengcomm, 12(5), 1391-1393 (2010).

54. M. A. Nadeem, M. Bhadbhade, R. Bircher, and J. A. Stride, Controlled Synthesis of Isomorphous Coordination Polymers via in Situ Ligand Transformation Reaction: Crystal Structure, Thermal and Magnetic Properties, Cryst. Growth Des., 10(9), 4060-4067 (2010).

55. M. A. Nadeem, M. Bhadbhade, and J. A. Stride, Four new coordination polymers constructed from benzene tricarboxylic acid: synthesis, crystal structure, thermal and magnetic properties, Dalton Trans., 39(41), 9860-9865 (2010).

56. M. A. Nadeem, D. J. Craig, R. Bircher, and J. A. Stride, Magneto-structural correlations of a three-dimensional Mn based metal-organic framework, 39(18), 4358-4362 (2010).

57. P. Niga, D. Wakeham, A. Nelson, G. G. Warr, M. Rutland, and R. Atkin, Structure of the Ethylammonium Nitrate Surface: An X-ray Reflectivity and Vibrational Sum Frequency Spectroscopy Study, Langmuir, 26(11), 8282-8288 (2010).

58. R. Nigam, A. V. Pan, S. X. Dou, S. J. Kennedy, A. J. Studer, and N. Stuesser, Magnetic field dependent neutron powder diffraction studies of $Ru_{0.9}Sr_2YCu_{2.1}O_{7.9}$, J. Appl. Phys., 107(9), 3 (2010).

59. T. H. Nguyen, T. Hanley, C. J. H. Porter, I. Larson, and B. J. Boyd, Phytantriol and glyceryl monooleate cubic liquid crystalline phases as sustained-release oral drug delivery systems for poorly water soluble drugs I. Phase behaviour in physiologically-relevant media, J. Pharm. Pharmacol., 62(7), 844-855 (2010).

60. T. H. Nguyen, T. Hanley, C. J. H. Porter, I. Larson, and B. J. Boyd, Phytantriol and glyceryl monooleate cubic liquid crystalline phases as sustained-release oral drug delivery systems for poorly water-soluble drugs II. In-vivo evaluation, J. Pharm. Pharmacol., 62(7), 856-865 (2010).

61. S. R. Olsen, S. A. Pullen, and M. Avdeev, A 100-position robotic sample changer for powder diffraction with low-background vacuum chamber, J. Appl. Crystallogr., 43, 377-379 (2010).

62. S. V. Patwardhan, S. A. Holt, S. M. Kelly, M. Kreiner, C. C. Perry and C. F. van der Walle, Silica Condensation by a Silicatein alpha Homologue Involves Surface-Induced Transition to a Stable Structural Intermediate Forming a Saturated Monolayer, Biomacromolecules 11, 3126-3135 (2010).

63. D. C. Pearce, K. Dowling, A. R. Gerson, M. R. Sim, S. R. Sutton, M. Newville, R. Russell, and G. McOrist, Arsenic microdistribution and speciation in toenail clippings of children living in a historic gold mining area, Sci. Total Environ., 408(12), 2590-2599 (2010).

64. V. K. Peterson, G. J. Kearley, Y. Wu, A. J. Ramirez-Cuesta, E. Kemner, and C. J. Kepert, Local Vibrational Mechanism for Negative Thermal Expansion: A Combined Neutron Scattering and First-Principles Study, Angew. Chem.-Int. Edit., 49(3), 585-588 (2010).

65. P. Photongkam, Y. B. Zhang, M. H. N. Assadi, S. Li, D. Yu, M. Ionescu, and A. V. Pan, Enhancement of Co substitution induced by Eu codoping in ZnO-based diluted magnetic semiconducting thin films, J. Appl. Phys., 107(3), Art. No. 033909 (2010).

66. A. Pramanick, A. D. Prewitt, M. A. Cottrell, W. Lee, A. J. Studer, K. An, C. R. Hubbard, and J. L. Jones, In situ neutron diffraction studies of a commercial, soft lead zirconate titanate ceramic: response to electric fields and mechanical stress, Appl. Phys. A-Mater. Sci. Process., 99(3), 557-564 (2010).

67. M. Rahlenbeck, M. Wagenknecht, A. Tsukada, D. Koelle, R. Kleiner, B. Keimer, and C. Ulrich, Raman light scattering study and microstructural analysis of epitaxial films of the electron-doped superconductor $La_{2-x}Ce_xCuO_4$, European Physical Journal B 75, 461-467 (2010).

68. S. Ramachandran, M. B. Taraban, J. Trewhella, I. Gryczynski, Z. Gryczynski, and Y. B. Yu, Effect of Temperature During Assembly on the Structure and Mechanical Properties of Peptide-Based Materials, Biomacromolecules, 11(6), 1502-1506 (2010).

69. A. Rekas, R. B. Knott, A. Sokolova, K. J. Barnham, K. A. Perez, C. L. Masters, S. C. Drew, R. Cappai, C. C. Curtain, and C. L. L. Pham, The structure of dopamine induced alpha-synuclein oligomers, Eur. Biophys. J. Biophys. Lett., 39(10), 1407-1419 (2010).

70. R. A. Ricciardo, H. L. Cuthbert, P. M. Woodward, Q. D. Zhou, B. J. Kennedy, Z. M. Zhang, M. Avdeev, and L. Y. Jang, Structure and Properties of $Sr_{1-x}Ca_xMn_{0.5}Ru_{0.5}O_3$ Perovskites: Using Chemical Pressure to Control Mn/Ru Mixed Valency, Chem. Mat., 22(11), 3369-3382 (2010).

71. T. Saerbeck, F. Klose, D. Lott, G. J. Mankey, Z. Lu, P. R. LeClair, W. Schmidt, A. P. J. Stampfl, S. Danilkin, M. Yethiraj, and A. Schreyer, Artificially modulated chemical order in thin films: A different approach to create ferro/antiferromagnetic interfaces, Phys. Rev. B, 82(13), Art. No. 134409 (2010).

72. P. J. Saines, J. R. Hester, and A. K. Cheetham, Neutron diffraction study of the magnetic structures of manganese succinate $Mn(C_4H_4O_4)$: A complex inorganic-organic framework, Phys. Rev. B, 82(14), Art. No. 144435 (2010).

73. N. V. Salim, T. Hanley, and Q. P. Guo, Microphase Separation through Competitive Hydrogen Bonding in Double Crystalline Diblock Copolymer/ Homopolymer Blends, Macromolecules, 43(18), 7695-7704 (2010).

74. T. Schmoelzer, K. D. Liss, G. A. Zickler, I. J. Watson, L. M. Droessler, W. Wallgram, T. Buslaps, A. Studer, and H. Clemens, Phase fractions, transition and ordering temperatures in TiAl-Nb-Mo alloys: An in- and ex-situ study, Intermetallics, 18(8), 1544-1552 (2010).

75. N. Sharma, R. B. Macquart, M. Avdeev, M. Christensen, G. J. McIntyre, Y. S. Chen, and C. D. Ling, Re-investigation of the structure and crystal chemistry of the Bi_2O_3-W_2O_6 'type (Ib)' solid solution using single-crystal neutron and synchrotron X-ray diffraction, Acta Crystallogr. Sect. B-Struct. Sci., 66, 165-172 (2010).

76. N. Sharma, V. K. Peterson, M. M. Elcombe, M. Avdeev, A. J. Studer, N. Blagojevic, R. Yusoff, and N. Kamarulzaman, Structural changes in a commercial lithium-ion battery during electrochemical cycling: An in situ neutron diffraction study, J. Power Sources, 195(24), 8258-8266 (2010).

77. A. K. Shrestha, C. S. Ng, A. Lopez-Rubio, J. Blazek, E. P. Gilbert, and M. J. Gidley, Enzyme resistance and structural organization in extruded high amylose maize starch, Carbohydr. Polym., 80(3), 699-710 (2010).

78. S. Siddiqui, A. Poljak, D. De Francisci, G. Guerriero, O. Pilak, D. Burg, M. J. Raftery, D. M. Parkin, J. Trewhella, and R. Cavicchioli, A chemically modified alpha-amylase with a molten-globule state has entropically driven enhanced thermal stability, Protein Eng. Des. Sel., 23(10), 769-780 (2010).

79. A. Sokolova, C. S. Kealley, T. Hanley, A. Rekas, and E. P. Gilbert, Small-Angle X-ray Scattering Study of the Effect of pH and Salts on 11S Soy Glycinin in the Freeze-Dried Powder and Solution States, J. Agric. Food Chem., 58(2), 967-974 (2010).

80. D. J. Sprouster, R. Giulian, L. L. Araujo, P. Kluth, B. Johannessen, D. J. Cookson, G. J. Foran, and M. C. Ridgway, Structural and vibrational properties of Co nanoparticles formed by ion implantation, J. Appl. Phys., 107(1), Art. No. 014313 (2010).

81. A. W. Stevenson, S. C. Mayo, D. Hausermann, A. Maksimenko, R. F. Garrett, C. J. Hall, S. W. Wilkins, R. A. Lewis, and D. E. Myers, First experiments on the Australian Synchrotron Imaging and Medical beamline, including investigations of the effective source size in respect of X-ray imaging, J. Synchrot. Radiat., 17, 75-80 (2010).

82. Y. L. Sun, D. D. Qu, Y. J. Sun, K. D. Liss, and J. Shen, Inhomogeneous structure and glass-forming ability in Zr-based bulk metallic glasses, J. Non-Cryst. Solids, 356(1), 39-45 (2010).

83. A. M. Telford, M. James, L. Meagher, and C. Neto, Thermally Cross-Linked PNVP Films As Antifouling Coatings for Biomedical Applications, ACS Appl. Mater. Interfaces, 2(8), 2399-2408 (2010).

84. G. J. Thorogood, M. Avdeev, and B. J. Kennedy, Structural studies of the aeschynite-euxenite transformation in the series $Ln(TiTa)O^{-}_{6}$ Ln = Lanthanide, Solid State Sci., 12(7), 1263-1269 (2010).

85. G. J. Thorogood, B. J. Kennedy, C. S. Griffith, M. M. Elcombe, M. Avdeev, J. V. Hanna, S. K. Thorogood, and V. Luca, Structure and Phase Transformations in the Titanosilicate, Sitinakite. The Importance of Water, Chem. Mater., 22(14), 4222-4231 (2010).

86. Ting, B. J. Kennedy, Z. Zhang, M. Avdeev, B. Johannessen, and L. Y. Jang, Synthesis and Structural Studies of the Transition-Metal-Doped Rh Perovskites $LaMn_{0.5}Rh_{0.5}O_3$ and $LaCu_{0.5}Rh_{0.5}O_3$, Chem. Mat., 22(5), 1640-1646 (2010).

87. T. M. Treweek, A. Rekas, M. J. Walker and J. A. Carver, A quantitative NMR spectroscopic examination of the flexibility of the C-terminal extensions of the molecular chaperones, alpha A- and alpha B-crystallin, Experimental Eye Research 91, 691-99 (2010).

88. B. H. Wang, J. M. Lawrence, A. D. Christianson, E. A. Goremychkin, V. R. Fanelli, K. Gofryk, E. D. Bauer, F. Ronning, J. D. Thompson, N. R. de Souza, A. I. Kolesnikov, and K. C. Littrell, Kondo behavior, ferromagnetic correlations, and crystal fields in the heavy-fermion compounds Ce_3X (X = In, Sn), Phys. Rev. B, 81(23), Art. No. 235132 (2010).

89. H. F. Wang, K. F. Cai, H. Li, D. H. Yu, X. Wang, C. W. Zhou, X. L. Li, Y. Y. Wang, B. J. An, and Y. Du, Synthesis and thermoelectric properties of single crystalline and polycrystalline $Ba_8Ga_{16}Ge_{30}$, J. Alloy. Compd., 491(1-2), 684-688 (2010).

90. N. A. S. Webster, I. C. Madsen, M. J. Loan, R. B. Knott, F. Naim, K. S. Wallwork, and J. A. Kimpton, An investigation of goethite-seeded $Al(OH)_3$ precipitation using in situ X-ray diffraction and Rietveld-based quantitative phase analysis, J. Appl. Crystallogr., 43, 466-472 (2010).

91. E. J. Wolfson, E. N. Caspi, H. Ettedgui, H. Shaked, and M. Avdeev, The effect of non-magnetic dilution of the Tb sublattice in $TbCo_3B_2$, J. Phys.-Condes. Matter, 22(2), Art. No. 026001 (2010).

92. K. Wood, D. J. Tobias, B. Kessler, F. Gabel, D. Oesterhelt, F. A. Mulder, G. Zaccai and M. Weik, The low-temperature inflection observed in neutron scattering measurements of proteins is due to methyl rotation: direct evidence using isotope labeling and molecular dynamics simulations, J. Am. Chem. Soc. 132, 4990-4991 (2010).

93. H. Wu, J. M. Simmons, Y. Liu, C. M. Brown, X. S. Wang, S. Ma, V. K. Peterson, P. D. Southon, C. J. Kepert, H. C. Zhou, T. Yildirim, and W. Zhou, Metal-Organic Frameworks with Exceptionally High Methane Uptake: Where and How is Methane Stored?, Chem.-Eur. J., 16(17), 5205-5214 (2010).

94. F. Xia, B. O'Neill, Y. Ngothai, J. Peak, C. Tenailleau, B. Etschmann, G. Qian, J. Brugger, A. Studer, S. Olsen, and A. Pring, A thermosyphon-driven hydrothermal flow-through cell for in situ and time-resolved neutron diffraction studies, J. Appl. Cryst., 43(3), 511-519 (2010).

95. F. Xia, G. Qian, J. Brugger, A. Studer, S. Olsen, and A. Pring, A large volume cell for in situ neutron diffraction studies of hydrothermal crystallizations, Rev. Sci. Instrum., 81(10), Art. No. 105107 (2010).

96. X. Xu, S. X. Dou, X. L. Wang, J. H. Kim, J. A. Stride, M. Choucair, W. K. Yeoh, R. K. Zheng, and S. P. Ringer, Graphene doping to enhance the flux pinning and supercurrent carrying ability of a magnesium diboride superconductor, Supercond. Sci. Technol., 23(8), Art. No. 085003 (2010).

97. K. Yan, D. G. Carr, M. D. Callaghan, K. D. Liss, and H. J. Li, Deformation mechanisms of twinning-induced plasticity steels: In situ synchrotron characterization and modeling, Scr. Mater., 62(5), 246-249 (2010).

98. H. Yee, T. Hanley, R. A. Evans, T. P. Davis, and G. E. Ball, Photochromic Spirooxazines Functionalized with Oligomers: Investigation of Core-Oligomer Interactions and Photomerocyanine Isomer Interconversion Using NMR Spectroscopy and DFT, J. Org. Chem., 75(9), 2851-2860 (2010).

99. S. I. Yun, V. Lo, J. Noorman, J. Davis, R. A. Russell, P. J. Holden, and G. E. Gadd, Morphology of composite particles of single wall carbon nanotubes/ biodegradable polyhydroxyalkanoates prepared by spray drying, Polym. Bull., 64(1), 99-106 (2010).

100. Zbiri, M. R. Johnson, L. Haverkate, F. M. Mulder and G. J. Kearley, "Molecular Modelling of Ground and Excited-States Vibrations in Organic Conducting Devices: Hexakis(n-hexytoxy)triphenylene (HAT6) as Case Study." Aus. J. Chem., 63(3), 388-395 (2010).

101. M. Zbiri, M. R. Johnson, G. J. Kearley, and F. M. Mulder, Density functional calculations of potential energy surface and charge transfer integrals in molecular triphenylene derivative HAT(6), Theor. Chem. Acc. 125, 445-451 (2010).

102. Q. D. Zhou, B. J. Kennedy, and M. Avdeev, Structural studies of the disorder and phase transitions in the double perovskite Sr_2YTaO_6, J. Solid State Chem., 183(8), 1741-1746 (2010)

2011

1. Andersen, KH; Bentley, PM and Cussen, LD, The ABC of powder diffractometer detector coverage, J. Appl. Crystallogr. 44, 295-298 (2011)

2. Anderson, KM; Goeta, AsE; Martin, JE; Mason, SA; McIntyre, GJ; Sansam, BCR; Wilkinson, C and Steed, JW, Dominance of Charge-Assisted Hydrogen Bonding on Short Contacts and Structures that Crystallize with Z' > 1, Cryst. Growth Des 11(11), 4904-4919 (2011)

3. Avdeev, M; Thorogood, GJ; Carter, ML; Kennedy, BJ; Ting, J; Singh, DJ and Wallwork, KS, Antiferromagnetism in a Technetium Oxide. Structure of $CaTcO_3$, J. Am. Chem. Soc. 133(6), 1654-1657 (2011) (from ECHIDNA)

4. Bartkowiak, M; Kearley, GJ; Yethiraj, M and Mulders, AM, Symmetry of ferroelectric phase of $SrTi_{18}O_3$ determined by ab initio calculations, Phys. Rev. B: Condens. Matter Mater. Phys. 83(6), Art. No. 064102 (2011) (from Computing Cluster)

5. Bartle, CM; Edgar, A; Dixie, L; Varoy, C; Piltz, R; Buchanan, S and Rutherford, K, Novel methods for measuring afterglow in developmental scintillators for X-ray and neutron detection, Nucl. Instrum. Methods Phys. Res., Sect. A 651(1), 105-109 (2011) (from Koala)

6. Beecham, CJ; Boag, S; Frost, CD; McKetterick, TJ; Stewart, JR; Andersen, KH; Bentley, PM and Jullien, D, ^{3}He polarization for ISIS TS2 phase I instruments, Phys. B 406(12), 2429-2432 (2011)

7. Bentley, PM; Fouquet, P; Bohm, M; Sutton, I; Dewhurst, CD and Andersen, KH, Global optimization of an entire neutron guide hall, J. Appl. Crystallogr. 44, 483-488 (2011)

8. Blazek, J and Gilbert, EP, Application of small-angle X-ray and neutron scattering techniques to the characterisation of starch structure: A review, Carbohydr. Polym. 85(2), 281-293 (2011) (from Bruker (SAXS))

9. Blazek, J; Gilbert, EP and Copeland, L, Effects of monoglycerides on pasting properties of wheat starch after repeated heating and cooling, J Cereal Sci 54(1), 151-159 (2011) (from Bruker (SAXS))

10. Bloch, ED; Murray, LJ; Queen, WL; Chavan, S; Maximoff, SN; Bigi, JP; Krishna, R; Peterson, VK; Grandjean, F; Long, GJ; Smit, B; Bordiga, S; Brown, CM and Long, JR, Selective Binding of O_2 over N_2 in a Redox-Active Metal-Organic Framework with Open Iron(II) Coordination Sites, J. Am. Chem. Soc. 133(37), 14814-14822 (2011) (from ECHIDNA)

11. Boeer, AB; Barra, AL; Chibotaru, LF; Collison, D; McInnes, EJL; Mole, RA; Simeoni, GG; Timco, GA; Ungur, L; Unruh, T and Winpenny, REP, A Spectroscopic Investigation of Magnetic Exchange Between Highly Anisotropic Spin Centers, Angew. Chem. Int. Ed. Engl. 50(17), 4007-4011 (2011)

12. Cadogan, JM; Avdeev, M; Kumar, P; Suresh, K and Ryan, DH, Neutron powder diffraction determination of the magnetic structure of Nd_2Al, J. Phys.: Conf. Ser. 303(1), Art. No. 012026 (2011) (from ECHIDNA)

13. Callaghan, MD; Humphries, SR; Law, M; Ho, M; Yan, K and Yeung, WY, Specimen-size dependency and modelling of energy evolution during high-temperature low-cycle fatigue of pressure vessel steel, Scr. Mater. 65(4), 308-311 (2011)

14. Cavaye, H; Shaw, PE; Smith, ARG; Burn, PL; Gentle, IR; James, M; Lo, S-C and Meredith, P, Solid State Dendrimer Sensors: Effect of Dendrimer Dimensionality on Detection and Sequestration of 2,4-Dinitrotoluene, J. Phys. Chem. C 115 (37), 18366-18371 (2011) (from PLATYPUS)

15. Chan, RTH; Garvey, CJ; Marçal, H; Russell, RA; Holden, PJ and Foster, LJR, Manipulation of Polyhydroxybutyrate Properties through Blending with Ethyl-Cellulose for a Composite Biomaterial, International Journal of Polymer Science 2011, Art. No. 651549 (2011)

16. Chan, RTH; Marçal, H; Russell, RA; Holden, PJ and Foster, LJR, Application of Polyethylene Glycol to Promote Cellular Biocompatibility of Polyhydroxybutyrate Films, International Journal of Polymer Science, Art. No. 473045 (2011)

17. Chan, WK; Haverkate, LA; Borghols, WJH; Wagemaker, M; Picken, SJ; van Eck, ERH; Kentgens, APM; Johnson, MR; Kearley, GJ and Mulder, FM, Direct View on Nanoionic Proton Mobility, Adv. Funct. Mater. 21(8), 1364-1374 (2011) (from Computing Cluster)

18. Ciampi, S; James, M; Darwish, N; Luais, E; Guan, B; Harper, JB and Gooding, JJ, Oxidative acetylenic coupling reactions as a surface chemistry tool, Phys. Chem. Chem. Phys. 13(34), 15624-15632 (2011) (from X-ray reflectometer)

19. Ciampi, S; James, M; Michaels, P and Gooding, JJ, Tandem "Click" Reactions at Acetylene-Terminated Si(100) Monolayers, Langmuir 27(11), 6940-6949 (2011) (from X-ray reflectometer)

20. Clements, R; Hester, JR; Kennedy, BJ; Ling, CD and Stampfl, APJ, The fluorite-pyrochlore transformation of $Ho_{2-y}Nd_yZr_2O_7$, J. Solid State Chem. 184(8), 2108–2113 (2011) (from ECHIDNA)

21. Cole, JM; Burgi, HB and McIntyre, GJ, Distinction of disorder, classical and quantum vibrational contributions to atomic mean-square amplitudes in dielectric pentachloronitrobenzene, Phys. Rev. B: Condens. Matter Mater. Phys. 83(22), Art. No. 224202 (2011)

22. Cortie, DL and Lewis, RA, Role of vanguard counter-potential in terahertz emission due to surface currents explicated by three-dimensional ensemble Monte Carlo simulation, Phys. Rev. B: Condens. Matter Mater. Phys. 84(15), Art. No. 15532 (2011)

23. Cortie, MB; Kealley, CS; Bhatia, V; Thorogood, GJ; Elcombe, MM and Avdeev, M, High temperature transformations of the $Au_7Cu_5Al_4$ shape-memory alloy, J. Alloy. Compd. 508(8), 3502-3508 (2011) (from ECHIDNA)

24. Crow, L; Robertson, L; Bilheux, H; Fleenor, M; Iverson, E; Tong, X; Stoica, D and Lee, WT, The CG1 instrument development test station at the high flux isotope reactor, Nucl. Instrum. Methods Phys. Res., Sect. A 634, S71-S74 (2011)

25. Danilkin, S; Avdeev, M; Sakuma, T; Macquart, R; Ling, C; Rusina, M and Izaola, Z, Neutron scattering study of short-range correlations and ionic diffusion in copper selenide, Ionics 17(1), 75-80 (2011) (from ECHIDNA)

26. Danilkin, SA; Avdeev, M; Sakuma, T; Macquart, R and Ling, CD, Neutron diffraction study of diffuse scattering in $Cu_{2-delta}$ Se superionic compounds, J. Alloy. Compd. 509(18), 5460-5465 (2011) (from ECHIDNA)

27. Darwish, TA; Evans, RA and Hanley, TL, Spiropyran, chromene and spirooxazine, mélange á trois: Molecular logic systems through selective and reversible deactivation of photochromism mediated by CO_2 gas, Dyes and Pigments 92(2), 817-824 (2011) (from NDF - Chemical Deuteration)

28. Darwish, TA; Evans, RA; James, M and Hanley, TL, Spiropyran–Amidine: A Molecular Canary for Visual Detection of Carbon Dioxide Gas, Chem.-Eur. J. 17(41), 11399-11404 (2011) (from NDF - Chemical Deuteration)

29. Deng, G; Pomjakushin, V; Petříček, V; Pomjakushina, E; Kenzelmann, M and Conder, K, Structural evolution of one-dimensional spin-ladder compounds $Sr_{14-x}Ca_xCu_{24}O_{41}$ with Ca doping and related evidence of hole redistribution, Phys. Rev. B: Condens. Matter Mater. Phys. 84(14), Art. No. 144111 (2011)

30. Deng, G; Radheep, DM; Thiyagarajan, R; Pomjakushina, E; Wang, S; Nikseresht, N; Arumugam, S and Conder, K, High oxygen pressure single crystal growth of highly Ca-doped spin ladder compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ (x>12), J. Cryst. Growth 327(1), 182-188 (2011)

31. Du, GD; Sharma, N; Peterson, VK; Kimpton, JA; Jia, DZ and Guo, ZP , Br-Doped $Li_4Ti_5O_{12}$ and Composite TiO2 Anodes for Li-ion Batteries: Synchrotron X-Ray and in situ Neutron Diffraction Studies, Adv. Funct. Mater. 21(20), 3990-3997 (2011) (from ECHIDNA, WOMBAT)

32. Dunstan, MT; Southon, PD; Kepert, CJ; Hester, J; Kimpton, JA and Ling, CD, Phase diagram, chemical stability and physical properties of the solid-solution $Ba_4Nb_{2-x}Ta_xO_9$, J. Solid State Chem. 184(10), 2648-2654 (2011) (from ECHIDNA)

33. Dutta, NK; Truong, MY; Mayavan, S; Choudhury, NR; Elvin, CM; Kim, M; Knott, R; Nairn, KM and Hill, AJ, A Genetically Engineered Protein Responsive to Multiple Stimuli, Angew. Chem. Int. Ed. Engl. 50(19), 4428-4431 (2011)

34. Edwards, AJ, Neutron Diffraction - Recent Applications to Chemical Structure Determination, Aus. J. Chem. 64(7), 869-872 (2011) (from Koala)

35. Ford, SJ; Delamore, OJ; Evans, JSO; McIntyre, GJ; Johnson, MR and Radosavljević Evans, I, Giant Deuteron Migration During the Isosymmetric Phase Transition in Deuterated 3,5-Pyridinedicarboxylic Acid, Chem.-Eur. J. 17(52), 14942-14951 (2011)

36. Freund, AK and Rehm, C, Phase space optimisation of the USANS instrument KOOKABURRA at the ANSTO OPAL reactor, Nucl. Instrum. Methods Phys. Res., Sect. A 634, S81-S89 (2011)

37. Freund, AK and Yu, DH, Optimisation and fabrication of a composite pyrolytic graphite monochromator for the PELICAN instrument at the ANSTO OPAL reactor, Nucl. Instrum. Methods Phys. Res., Sect. A 634, S75-S80 (2011)

38. Fuentes-Montero, L; Montero-Cabrera, ME and Fuentes-Cobas, L, The software package ANAELU for X-ray diffraction analysis using two-dimensional patterns, J. Appl. Crystallogr. 44, 241-246 (2011)

39. Gardberg, AS; Potter, BS; Palmer, RA; McIntyre, GJ and Myles, DAA, The Neutron Structure of the Formyl Peptide Receptor Antagonist Cyclosporin H (CsH) Unambiguously Determines the Solvent and Hydrogen-Bonding Structure for Crystal Form II, J. Chem. Crystallogr. 41, 470-480 (2011)

40. Gatta, GD; McIntyre, GJ; Sassi, R; Rotiroti, N and Pavese, A, Hydrogen-bond and cation partitioning in muscovite: A single-crystal neutron-diffraction study at 295 and 20 K, Am. Mineral. 96(2), 34-41 (2011)

41. Grage, SL; Keleshian, AM; Turdzeladze, T; Battle, AR; Tay, WC; May, RP; Holt, SA; Contera, SA; Haertlein, M; Moulin, M; Pal, P; Rohde, PR; Forsyth, VT; Watts, A; Huang, KC; Ulrich, AS and Martinac, B, Bilayer-Mediated Clustering and Functional Interaction of MscL Channels, Biophys. J. 100(5), 1252-1260 (2011)

42. Griffith, MJ; James, M; Triani, G; Wagner, P; Wallace, GG and Officer, DL, Determining the Orientation and Molecular Packing of Organic Dyes on a TiO_2 Surface Using X-ray Reflectometry, Langmuir 27(21), 12944-12950 (2011) (from X-ray reflectometer)

43. Gummow, RJ; Sharma, N; Peterson, VK and He, Y, Synthesis, structure, and electrochemical performance of magnesium-substituted lithium manganese orthosilicate cathode materials for lithium-ion batteries, J. Power Sources 197, 231-237 (2011) (from ECHIDNA, WOMBAT)

44. He, LZ; Onaizi, SA; Dimitrijev-Dwyer, M; Malcolm, AS; Shen, HH; Dong, CC; Holt, SA; Thomas, RK and Middelberg, APJ, Comparison of positional surfactant isomers for displacement of rubisco protein from the air-water interface, J. Colloid Interface Sci. 360(2), 617-622 (2011)

45. Hudspeth, JM; Stewart, GA; Studer, AJ and Goossens, DJ, Crystal and magnetic structures in Perovskite-related La(1-x) Ca(x)FeO(3-delta) (x=0.2, 0.33), J. Phys. Chem. Solids 72(12), 1543-1547 (2011) (from WOMBAT)

46. Huson, MG; Strounina, EV; Kealley, CS; Rout, MK; Church, JS; Appelqvist, IAM; Gidley, MJ and Gilbert, EP, Effects of Thermal Denaturation on the Solid-State Structure and Molecular Mobility of Glycinin, Biomacromolecules 12(6), 2092-2102 (2011) (from Bruker (SAXS))

47. Jacques, DA; Langley, DB; Hynson, RMG; Whitten, AE; Kwan, A; Guss, JM and Trewhella, J, A Novel Structure of an Antikinase and its Inhibitor, J. Mol. Biol. 405(1), 214-226 (2011)

48. Jacques, DA; Langley, DB; Kuramitsu, S; Yokoyama, S; Trewhella, J and Guss, JM, The structure of TTHA0988 from Thermus thermophilus, a KipI-KipA homologue incorrectly annotated as an allophanate hydrolase, Acta Crystallographica Section D-Biological Crystallography 67, 105-111 (2011)

49. James, M; Ciampi, S; Darwish, TA; Hanley, TL; Sylvester, SO and Gooding, JJ , Nanoscale Water Condensation on Click-Functionalized Self-Assembled Monolayers, Langmuir 27(17), 10753-10762 (2011) (from X-ray reflectometer)

50. James, M; Darwish, TA; Ciampi, S; Sylvester, SO; Zhang, Z; Ng, A; Gooding, JJ and Hanley, TL, Nanoscale Condensation of Water on Self-Assembled Monolayers, Soft Matter 7(11), 5309–5318 (2011) (from PLATYPUS, X-ray reflectometer)

51. James, M; Nelson, A; Holt, SA; Saerbeck, T; Hamilton, WA and Klose, F, The multipurpose time-of-flight neutron reflectometer “PLATYPUS” at Australia’s OPAL reactor, Nucl. Instrum. Methods Phys. Res., Sect. A 632(1), 112-123 (2011) (from PLATYPUS)

52. Jeffries, CM; Lu, YL; Hynson, RMG; Taylor, JE; Ballesteros, M; Kwan, AH and Trewhella, J, Human Cardiac Myosin Binding Protein C: Structural Flexibility within an Extended Modular Architecture, J. Mol. Biol. 414(5), 735-748 (2011)

53. Johansen, D; Jeffries, CMJ; Hammouda, B; Trewhella, J and Goldenberg, DP, Effects of Macromolecular Crowding on an Intrinsically Disordered Protein Characterized by Small-Angle Neutron Scattering with Contrast Matching, Biophys. J. 100(4), 1120-1128 (2011)

54. Kabra, S; Yan, K; Mayer, S; Schmoelzer, T; Reid, M; Dippenaar, R; Clemens, H; and Liss, KD, Phase transition and ordering behavior of ternary Ti-Al-Mo alloys using in-situ neutron diffraction, International Journal of Materials Research 102(6), 697-702 (2011) (from WOMBAT)

55. Kawaguchi, D; Nelson, A; Masubuchi, Y; Majewski, JP; Torikai, N; Yamada, NL; Sarah, ARS; Takano, A and Matsushita, Y, Precise Analyses of Short-Time Relaxation at Asymmetric Polystyrene Interface in Terms of Molecular Weight by Time-Resolved Neutron Reflectivity Measurements, Macromolecules 44(23), 9424-9433 (2011)

56. Kennedy, BJ and Avdeev, M, The Structure of C-type Gd_2O_3. A Powder Neutron Diffraction Study using Enriched Gd-160, Aus. J. Chem. 64(1), 119-121 (2011) (from ECHIDNA)

57. Kennedy, BJ; Zhou, QD and Avdeev, M, Neutron diffraction studies of $Gd_2Zr_2O_7$ pyrochlore, J. Solid State Chem. 184(7), 1695-1698 (2011) (from ECHIDNA)

58. Kennedy, BJ; Zhou, QD and Avdeev, M, The ferroelectric phase of $CdTiO_3$: A powder neutron diffraction study, J. Solid State Chem. 184(11), 2987-2993 (2011) (from ECHIDNA)

59. Kirstein, O; Zhang, JF; Kisi, EH and Riley, DP, Ab Initio Phonon Dispersion Curves Used to Check Experimentally Determined Elastic Constants of the MAX Phase Ti_3SiC_2, Adv. Mater. Res. 275, 135-138 (2011) (from Computing Cluster)

60. Kjallman, THM; Nelson, A; James, M; Dura, JA; Travas-Sejdic, J and McGillivray, DJ, A neutron reflectivity study of the interfacial and thermal behaviour of surface-attached hairpin DNA, Soft Matter 7(10), 5020-5029 (2011) (from PLATYPUS, X-ray reflectometer)

61. Koo, HJ; Lee, C; Whangbo, MH; McIntyre, GJ and Kremer, RK, On the Nature of the Spin Frustration in the CuO_2 Ribbon Chains of $LiCuVO_4$: Crystal Structure Determination at 1.6 K, Magnetic Susceptibility Analysis, and Density Functional Evaluation of the Spin Exchange Constants, Inorg. Chem. 50(8), 3582-3588 (2011)

62. Kuperkar, KC; Mata, JP and Bahadur, P, Effect of 1-alkanols/salt on the cationic surfactant micellar aqueous solutions-A dynamic light scattering study, Colloid Surface A 380(1-3), 60-65 (2011)

63. Law, M and Luzin, V, Effect of spatial variation of stress-free lattice spacings on measured residual stresses, Journal of Strain Analysis for Engineering Design 46(8), 837-841 (2011) (from KOWARI)

64. Le Brun, AP; Holt, SA; Shah, DSH; Majkrzak, CF and Lakey, JH, The structural orientation of antibody layers bound to engineered biosensor surfaces, Biomaterials 32(12), 3303-3311 (2011)

65. Le Brun, AP; Shah, DSH; Athey, D; Holt, SA and Lakey, JH, Self-Assembly of Protein Monolayers Engineered for Improved Monoclonal Immunoglobulin G Binding, Int. J. Mol. Sci. 12(8), 5157-5167 (2011)

66. Lee, KH; Schwenn, PE; Smith, ARG; Cavaye, H; Shaw, PE; James, M; Krueger, KB; Gentle, IR; Meredith, P and Burn, PL, Morphology of all-solution-processed bilayer organic solar cells, Adv. Mater. 23(6), 766-770 (2011) (from PLATYPUS)

67. Li, XL; Cai, KF; Yu, DH and Wang, YY, Electrodeposition and characterization of thermoelectric Bi_2Te_2Se/Te multilayer nanowire arrays, Superlattice Microst 50(5), 557-562 (2011)

68. Liu, J; Yuan, L; Yang, X; Elbert, A and Harris, AT, Synthesis of vertically aligned carbon nanotube arrays on polyhedral Fe/Al_2O_3 catalysts, Chem. Commun. 47(22), 6434-6436 (2011)

69. Lu, YL; Jeffries, CM and Trewhella, J, Probing the Structures of Muscle Regulatory Proteins Using Small-Angle Solution Scattering, Biopolymers 95(8), 505-516 (2011)

70. Luzin, V; Spencer, K and Zhang, MX, Residual stress and thermo-mechanical properties of cold spray metal coatings, Acta Mater. 59(3), 1259-1270 (2011) (from ECHIDNA, KOWARI)

71. Marsilius, M; Granzowa, T and Jones, JL, Quantitative comparison between the degree of domain orientation and nonlinear properties of a PZT ceramic under electrical and mechanical loading, J. Mater. Res. 26(9), 1126-1132 (2011) (from KOWARI)

72. Mata, JP; Udabage, P and Gilbert, EP, Structure of casein micelles in milk protein concentrate powders via small angle X-ray scattering, Soft Matter 7(8), 3837-3843 (2011) (from Bruker (SAXS))

73. Miao, MH; Hawkins, SC; Cai, JY; Gengenbach, TR; Knott, R and Huynh, CP, Effect of gamma-irradiation on the mechanical properties of carbon nanotube yarns, Carbon 49(14), 4940-4947 (2011)

74. Mihalik, M; Prokleška, J; Kamarád, J; Prokescaron, K; Isnard, O; McIntyre, GJ; Dönni, A; Yoshii, S; Kitazawa, H; Sechovský, V and de Boer, FR, NdRhSn: A ferromagnet with an antiferromagnetic precursor, Phys. Rev. B: Condens. Matter Mater. Phys. 83(10), Art. No.104403 (2011)

75. Miiller, W; Avdeev, M; Zhou, Q; Studer, AJ; Kennedy, BJ; Kearley, GJ and Ling, CD, Spin-gap opening accompanied by a strong magnetoelastic response in the S=1 magnetic dimer system $Ba_3BiRu_2O_9$, Phys. Rev. B: Condens. Matter Mater. Phys. 84(22), Art. No. 220406 (2011) (from Computing Cluster, WOMBAT)

76. Miiller, W; Christensen, M; Khan, A; Sharma, N; Macquart, RB; Avdeev, M; McIntyre, GJ; Piltz, RO and Ling, CD, $YCa_3(VO)_3(BO_3)_4$: A Kagome Compound Based on Vanadium(III) with a Highly Frustrated Ground State, Chem. Mater. 23(5), 1315-1322 (2011) (from ECHIDNA, Koala)

77. Minakshi, M; Sharma, N; Ralph, D; Appadoo, D and Nallathamby, K, Synthesis and Characterization of $Li(Co_{0.5}Ni_{0.5})$ PO4 Cathode for Li-Ion Aqueous Battery Applications, Electrochem. Solid-State Lett. 14(6), A86-A89 (2011) (from ECHIDNA)

78. Minakshi, M; Singh, P; Sharma, N; Blackford, M and Ionescu, M, Lithium Extraction-Insertion from/into $LiCoPO_4$ in Aqueous Batteries, Ind. Eng. Chem. Res. 50(4), 1899-1905 (2011)

79. Mole, RA; Stride, JA; Henry, PF; Hoelzel, M; Senyshyn, A; Alberola, A; Garcia, CJG; Raithby, PR and Wood, PT, Two Stage Magnetic Ordering and Spin Idle Behavior of the Coordination Polymer Co-3(OH)(2) (C_4O_4)(2)center dot 3H(2)O Determined Using Neutron Diffraction, Inorg. Chem. 50(6), 2246-2251 (2011)

80. Mulders, AM; Bartkowiak, M; Hester, JR; Pomjakushina, E and Conder, K, Ferroelectric charge order stabilized by antiferromagnetism in multiferroic $LuFe_2O_4$, Phys. Rev. B: Condens. Matter Mater. Phys. 84(14), Art. No. 140403 (2011) (from WOMBAT)

81. Nadeem, MA; Thornton, AW; Hill, MR and Stride, JA, A flexible copper based microporous metal-organic framework displaying selective adsorption of hydrogen over nitrogen, Dalton Trans. 40(13), 3398-3401 (2011)

82. Noked, O; Yakovlev, S; Greenberg, Y; Garbarino, G; Shuker, R; Avdeev, M and Sterer, E, Pressure-induced amorphization of La(1/3)NbO_3, J. Non-Cryst. Solids 357(18), 3334-3337 (2011)

83. Ouladdiaf, B; Archer, J; Allibon, JR; Decarpentrie, P; Rodriguez-Carvajal, J; Lemée-Cailleau, MH; Hewat, AW: York, S; Brau, D and McIntyre, GJ, CYCLOPS - a reciprocal-space explorer based on CCD neutron detectors, J. Appl. Crystallogr. 44, 392-397 (2011)

84. Pang, WK; Low, IM; O'Connor, BH; Peterson, VK; Studer, AJ and Palmquist, JP, In situ diffraction study of thermal decomposition in Maxthal Ti_2AlC, J. Alloy. Compd. 509(1), 172-176 (2011) (from ECHIDNA, WOMBAT)

85. Pappas, C; Lelievre-Berna, E; Bentley, P; Falus, P; Fouquet, P and Farago, B, Magnetic fluctuations and correlations in MnSi: Evidence for a chiral skyrmion spin liquid phase, Phys. Rev. B: Condens. Matter Mater. Phys. 83(22), Art. No. 224405 (2011)

86. Paskevicius, M; Sheppard, DA; Chaudhary, AL; Webb, CJ; Gray, EMA; Tian, HY; Peterson, VK and Buckley, CE, Kinetic limitations in the Mg-Si-H system, Int. J. Hydrogen Energy 36(17), 10779-10786 (2011) (from WOMBAT)

87. Patwardhan, SV; Holt, SA; Kelly, SM; Kreiner, M; Perry, CC and van der Walle, CF, Silica Condensation by a Silicate in alpha Homologue Involves Surface-Induced Transition to a Stable Structural Intermediate Forming a Saturated Monolayer, Biomacromolecules 11(11), 3126-3135 (2011)

88. Peterson, VK; Brown, CM; Liu, Y and Kepert, CJ, Structural Study of D-2 within the Trimodal Pore System of a Metal Organic Framework, J. Phys. Chem. C 115(17), 8851-8857 (2011)

89. Peterson, VK; Shoko, E and Kearley, GJ, The effect of host relaxation and dynamics on guest molecule dynamics in H_2/tetrahydrofuran-hydrate, Faraday Discuss. 151, 37-46 (2011) (from Computing Cluster)

90. Phan, S; Fong, WK; Kirby, N; Hanley, T and Boyd, BJ, Evaluating the link between self-assembled mesophase structure and drug release, Int. J. Pharm. 421(1), 176-182 (2011)

91. Pojprapai, S; Simons, H; Studer, AJ; Luo, Z and Hoffman, M, Temperature Dependence on Domain Switching Behavior in Lead Zirconate Titanate Under Electrical Load via In Situ Neutron Diffraction, J. Am. Ceram. Soc. 94(10), 3202-3205 (2011) (from WOMBAT)

92. Princep, AJ; Mulders, AM; Staub, U; Scagnoli, V; Nakamura, T; Kikkawa, A; Lovesey, SW and Balcar, E, Triakontadipole and high-order dysprosium multipoles in the antiferromagnetic phase of DyB_2C_2, J. Phys.: Condens. Matter 23(26), Art. No. 266002 (2011)

93. Qasim, I; Kennedy, BJ; Zhang, ZM; Avdeev, M and Jang, LY, X-ray absorption near edge structure and crystallographic studies of the mixed valence oxide SrRu(0.8)Ni(0.2)O(3), J. Phys.: Condens. Matter 23(43), Art. No. 435401 (2011) (from ECHIDNA)

94. Qu, DD; Liss, KD; Yan, K; Reid, M; Almer, JD; Wang, YB; Liao, XZ and Shen, J, On the Atomic Anisotropy of Thermal Expansion in Bulk Metallic Glass, Adv. Eng. Mater. 13(9), 861-864 (2011)

95. Queen, WL; Brown, CM; Britt, DK; Zajdel, P; Hudson, MR and Yaghi, OM, Site-Specific CO_2 Adsorption and Zero Thermal Expansion in an Anisotropic Pore Network, J. Phys. Chem. C 115(50), 24915-24919 (2011)

96. Randau, C; Garbe, U and Brokmeier, HG, StressTextureCalculator: a software tool to extract texture, strain and microstructure information from area-detector measurements, J. Appl. Crystallogr. 44, 641-646 (2011)

97. Ratcliff, W; Kan, D; Chen, WC; Watson, S; Chi, SX; Erwin, R; McIntyre, GJ; Capelli, SC and Takeuchi, I, Neutron Diffraction Investigations of Magnetism in $BiFeO_3$ Epitaxial Films, Adv. Funct. Mater. 21(9), 1567-1574 (2011)

98. Reddy, MV; Raju, MJS; Sharma, N; Quan, PY; Nowshad, SH; Emmanuel, HEC; Peterson, VK and Chowdari, BVR, Preparation of $Li_{1.03}Mn_{1.97}O_4$ and $Li_{1.06}Mn_{1.94}O_4$ by the Polymer Precursor Method and X-ray, Neutron Diffraction and Electrochemical Studies, J. Electrochem. Soc. 158(11), A1231-A1236 (2011) (from WOMBAT)

99. Reehuis, M; Ulrich, C; Prokeš, K; Mat'aš, S; Fujioka, J; Miyasaka, S; Tokura, Y and Keimer, B, Structural and magnetic phase transitions of the orthovanadates RVO_3 (R= Dy, Ho, Er) as seen via neutron diffraction, Phys. Rev. B: Condens. Matter Mater. Phys. 83(6), Art. No. 064404 (2011)

100. Ricco, M; Pontiroli, D; Mazzani, M; Choucair, M; Stride, JA and Yazyev, OV, Muons Probe Strong Hydrogen Interactions with Defective Graphene, Nano Lett. 11(11), 4919-4922 (2011)

101. Rodriguez, DM; Kennedy, SJ and Bentley, PM, Properties of elliptical guides for neutron beam transport and applications for new instrumentation concepts, J. Appl. Crystallogr. 44, 727-737 (2011)

102. Rodriguez, EE; Poineau, F; Llobet, A; Kennedy, BJ; Avdeev, M; Thorogood, GJ; Carter, ML; Seshadri, R; Singh, DJ and Cheetham, AK, High Temperature Magnetic Ordering in the 4d Perovskite $SrTcO_3$, Phys. Rev. Lett. 106(6), Art. No. 067201 (2011) (from ECHIDNA)

103. Saerbeck, T; Loh, N; Lott, D; Toperverg, BP; Mulders, AM; Rodriguez, AF; Freeland, JW; Ali, M; Hickey, BJ; Stampfl, APJ; Klose, F and Stamps, RL, Spatial Fluctuations of Loose Spin Coupling in CuMn/Co Multilayers, Phys. Rev. Lett. 107(12), 7201-7201 (2011)

104. Saines, PJ; Yeung, HHM; Hester, JR; Lennie, AR and Cheetham, AK, Detailed investigations of phase transitions and magnetic structure in Fe(iii), Mn(ii), Co(ii) and Ni(ii) 3,4,5-trihydroxybenzoate (gallate) dihydrates by neutron and X-ray diffraction, Dalton Trans. 40(24), 6401-6410 (2011) (from ECHIDNA)

105. Salamakha, L; Bauer, E; Michor, H; Hilscher, G; Muller, H; Svagera, R; Sologub, O; Rogl, P; Hester, J; Roisnel, T; Giester, G and Mudryi, S, First-Order Phase Transition in a New $CaCu_5$-Related Antimonide, $CePt_5Sb$, Chem. Mater. 23(17), 4016-4024 (2011) (from ECHIDNA)

106. Schmoelzer, T; Liss, KD; Staron, P; Mayer, S and Clemens, H, The Contribution of High-Energy X-Rays and Neutrons to Characterization and Development of Intermetallic Titanium Aluminides, Adv. Eng. Mater. 13(8), 685-699 (2011) (from WOMBAT)

107. Schmoelzer, T; Mayer, S; Sailer, C; Haupt, F; Guther, V; Staron, P; Liss, KD and Clemens, H, In Situ Diffraction Experiments for the Investigation of Phase Fractions and Ordering Temperatures in Ti-44 at% Al-(3-7) at% Mo Alloys, Adv. Eng. Mater. 13(4), 306-311 (2011)

108. Schokker, EP; Church, JS; Mata, JP; Gilbert, EP; Puvanenthiran, A and Udabage, P, Reconstitution properties of micellar casein powder: Effects of composition and storage, Int. Dairy J. 21(11), 877-886 (2011)

109. Shamba, P; Debnath, JC; Zeng, R; Wang, JL; Campbell, SJ; Kennedy, SJ and Dou, SX, Reduction of hysteresis losses in the magnetic refrigerant $La_{0.8}Ce_{0.2}Fe_{11.4}Si_{1.6}$ by the addition of boron, J. Appl. Phys. 109(7), Art. No. 07a940 (2011)

110. Sharma, N; Du, G; Studer, AJ; Guo, Z and Peterson, VK, In-situ neutron diffraction study of the MoS_2 anode using a custom-built Li-ion battery, Solid State Ionics 199-200, 37-43 (2011) (from WOMBAT)

111. Sharma, N; Reddy, MV; Du, G; Adams, S; Chowdari, BVR; Guo, Z and Peterson, VK, Time-Dependent in-Situ Neutron Diffraction Investigation of a $Li(Co_{0.16}Mn_{1.84})O_4$ Cathode, J. Phys. Chem. C 115(43), 21473-21480 (2011) (from ECHIDNA, WOMBAT)

112. Shen, H-H; Hartley, PG; James, M; Nelson, A; Defendi, H and McLean, KM, The interaction of cubosomes with supported phospholipid bilayers using neutron reflectometry and QCM-D , Soft Matter 7(18), 8041–8049 (2011) (from PLATYPUS)

113. Shima, T; Luo, Y; Stewart, T; Bau, R; McIntyre, GJ; Mason, SA and Hou, Z, Molecular heterometallic hydride clusters composed of rare-earth and d-transition metals, Nat. Chem. 3(10), 814-820 (2011)

114. Shoko, E; Smith, MF and McKenzie, RH, Charge distribution and transport properties in reduced ceria phases: A review, J. Phys. Chem. Solids 72(12), 1482-1494 (2011)

115. Simons, H; Daniels, J; Jo, W; Dittmer, R; Studer, A; Avdeev, M; Rodel, J and Hoffman, M, Electric-field-induced strain mechanisms in lead-free 94%$(Bi_{1/2}Na_{1/2})TiO_3$-6%$BaTiO_3$, Appl. Phys. Lett. 98(8), Art. No. 082901 (2011) (from ECHIDNA)

116. Smith, ARG; Ruggles, JL; Cavaye, H; Shaw, PE; Darwish, TA; James, M; Gentle, IR and Burn, PL, Investigating Morphology and Stability of Fac-tris (2-phenylpyridyl) iridium(III) Films for OLEDs, Adv. Funct. Mater. 21(12), 2225-2231 (2011) (from NDF - Chemical Deuteration, PLATYPUS)

117. Solanki, RS; Singh, AK; Mishra, SK; Kennedy, SJ; Suzuki, T; Kuroiwa, Y; Moriyoshi, C and Pandey, D, Ground state of $(Pb_{0.94}Sr_{0.06})(Zr_{0.530}Ti_{0.470})O_3$ in the morphotropic phase boundary region: Evidence for a monoclinic Cc space group, Phys. Rev. B: Condens. Matter Mater. Phys. 84(14), Art. No. 144116 (2011) (from ECHIDNA, WOMBAT)

118. Taraban, MB; Ramachandran, S; Gryczynski, I; Gryczynski, Z; Trewhella, J and Yu, YHB, Effects of chain length on oligopeptide hydrogelation, Soft Matter 7(6), 2624-2631 (2011)

119. Telford, AM; Thickett, SC; James, M and Neto, C, Competition between Dewetting and Cross-Linking in Poly(N-vinylpyrrolidone)/Polystyrene Bilayer Films, Langmuir 27(23), 14207-14217 (2011) (from PLATYPUS)

120. Thorogood, GJ; Avdeev, M; Carter, ML; Kennedy, BJ; Ting, J and Wallwork, KS, Structural phase transitions and magnetic order in $SrTcO_3$, Dalton Trans. 40(27), 7228-7233 (2011) (from ECHIDNA)

121. Thorogood, GJ; Kennedy, BJ; Avdeev, M; Peterson, VK; Hanna, JV and Luca, V, Cation disorder in $NaW_2O_{6+\delta}.nH_{2-z}O$ post ion exchange with K, Rb, Sr, and Cs, J. Phys. Chem. Solids 72(6), 692-700 (2011) (from ECHIDNA)

122. Thorogood, GJ; Orain, P-Y; Ouvry, M; Piriou, B; Tony, T; Wallwork, KS; Herrmann, J and James, M, Structure, Crystal Chemistry And Magnetism Of Rare Earth Calcium-Doped Cobaltates: $Ln_{2-x}Ca_xCoO_{4+d}$ (Ln = Pr, Nd, Sm, Eu And Gd), Solid State Sci 13(12), 2113-2123 (2011)

123. Thorogood, GJ; Zhang, ZM; Hester, JR; Kennedy, BJ; Ting, J; Glover, CJ and Johannessen, B, Structure and cation ordering in spinel-type $TcCo_2O_4$. An example of a trivalent technetium oxide, Dalton Trans. 40(41), 10924-10926 (2011) (from WOMBAT)

124. Toudic, B; Rabiller, P; Bourgeois, L; Huard, M; Ecolivet, C; McIntyre, GJ; Bourges, P; Breczewski, T and Janssen, T, Temperature-pressure phase diagram of an aperiodic host guest compound, Europhysics Letters 93(1), Art. No.16003 (2011)

125. Velinov, T; Ahtapodov, L; Nelson, A; Gateshki, M and Bivolarska, M, Influence of the surface roughness on the properties of Au films measured by surface plasmon resonance and X-ray reflectometry, Thin Solid Films 519(7), 2093-2097 (2011) (from X-ray reflectometer)

126. Wacklin, HP, Composition and Asymmetry in Supported Membranes Formed by Vesicle Fusion, Langmuir 27(12), 7698-7707 (2011)

127. Wagemaker, M; Singh, D. P; Borghols, W. J.H; Lafont, U; Haverkate, L; Peterson, V. K and Mulder, F. M, Dynamic Solubility Limits in Nanosized Olivine $LiFePO_4$, J. Am. Chem. Soc. 133(26), 10222–10228 (2011) (from WOMBAT)

128. Wagner, K; Griffith, MJ; James, M; Mozer, AJ; Wagner, P; Triani, G; Officer, DL and Wallace, GG, Significant Performance Improvement of Porphyrin-Sensitized TiO_2 Solar Cells under White Light Illumination, J. Phys. Chem. C 115(1), 317-326 (2011) (from X-ray reflectometer)

129. Wakeham, D; Nelson, A; Warr, GG and Atkin, R, Probing the protic ionic liquid surface using X-ray reflectivity, Phys. Chem. Chem. Phys. 13(46), 20828-20835 (2011) (from X-ray reflectometer)

130. Wang, J; Liu, Y; Withers, RL; Studer, A; Li, Q; Norén, L and Guo, Y , A correlated electron diffraction, in situ neutron diffraction and dielectric properties investigation of poled $(1-x)Bi_{0.5}Na_{0.5}TiO_{3-x}BaTiO_3$ ceramics, J. Appl. Phys. 110(8), Art. No. 084114 (2011) (from WOMBAT)

131. Wang, JL; Campbell, SJ; Cadogan, JM; Studer, AJ; Zeng, R and Dou, SX, Magnetocaloric effect in layered $NdMn_2Ge_{0.4}Si_{1.6}$, Appl. Phys. Lett. 98(23), Art. No. 232509 (2011) (from WOMBAT)

132. Wang, JL; Campbell, SJ; Cadogan, JM; Studer, AJ; Zeng, R and Dou, SX, Neutron diffraction study of the magnetic order in $NdMn_2Ge_{1.6}Si_{0.4}$, J. Phys.: Conf. Ser. 303(1), Art. No. 012022 (2011) (from WOMBAT)

133. Wang, JL; Campbell, SJ; Kennedy, SJ; Zeng, R; Dou, SX and Wu, GH, Critical magnetic transition in $TbNi_2Mn$-magnetization and Mössbauer spectroscopy, J. Phys.: Condens. Matter 23(21), Art. No. 216002 (2011) (from WOMBAT)

134. Wang, JL; Campbell, SJ; Zeng, R; Dou, SX and Kennedy, SJ, Magnetic phase transition and Mossbauer spectroscopy of $ErNi_2Mn_x$ compounds, J. Appl. Phys. 109(7), 07E304 (2011) (from WOMBAT)

135. Wang, JL; Studer, AJ; Campbell, SJ; Kennedy, SJ; Zeng, R; Dou, SX and Wu, GH, Magnetic Structures of $Pr_{0.8}Lu_{0.2}Mn_2Ge_2$ and $Pr_{0.6}Lu_{0.4}Mn_2Ge_2$, IEEE Transactions on Magnetics 47(10), 2893-2896 (2011) (from WOMBAT)

136. Wang, SH; Sun, YS; Chiang, AST; Hung, HF; Chen, MC and Wood, K, Carboxylic Acid-Directed Clustering and Dispersion of ZrO_2 Nanoparticles in Organic Solvents: A Study by Small-Angle X-ray/Neutron Scattering and NMR, J. Phys. Chem. C 115(24), 11941-11950 (2011) (from QUOKKA)

137. Webster, NAS; Hartlieb, KJ; Saines, PJ; Ling, CD and Lincoln, FJ, New quenched-in fluorite-type materials in the Bi_2O_3-La_2O_3-PbO system: Synthesis and complex phase behaviour up to 750 degrees C, Mater. Res. Bull. 46(4), 538-542 (2011)

138. Webster, NAS; Loan, MJ; Madsen, IC; Knott, RB and Kimpton, JA, An investigation of the mechanisms of goethite, hematite and magnetite-seeded $Al(OH)_3$ precipitation from synthetic Bayer liquor, Hydrometallurgy 109(1-2), 72-79 (2011)

139. Weir, MP and Parnell, AJ, Water Soluble Responsive Polymer Brushes, Polymers 3(4), 2107-2132 (2011)

140. Weir, MP; Heriot, SY; Martin, SJ; Parnell, AJ; Holt, SA; Webster, JRP and Jones, RAL, Voltage-Induced Swelling and Deswelling of Weak Polybase Brushes, Langmuir 27(17), 11000-11007 (2011)

141. White, CE; Provis, JL; Kearley, GJ; Riley, DP and van Deventer, JSJ, Density functional modelling of silicate and aluminosilicate dimerisation solution chemistry, Dalton Trans. 40(6), 1348-1355 (2011) (from Computing Cluster)

142. Whitfield, R; Studer, A and Goossens, D, Temperature Dependence of Diffuse Scattering in PZN, Metall. Mater. Trans. A 43(5), 1429-1433 (2011) (from WOMBAT)

143. Yamada, M; Iwashita, Y; Kanaya, T; Ichikawa, M; Tongu, H; Kennedy, SJ; Shimizu, HM; Mishima, K; Yamada, NL; Hirota, K; Carpenter, JM; Lal, J; Andersen, K; Geltenbort, P; Guerard, B; Manzin, G; Hino, M; Kitaguchi, M and Bleuel, M, The performance of magnetic lens for focusing VCN-SANS, Nucl. Instrum. Methods Phys. Res., Sect. A 634, S156-S160 (2011)

144. Yan, K; Carr, DG; Kabra, S; Reid, M; Studer, A; Harrison, RP; Dippenaar, R and Liss, K-D, In Situ Characterization of Lattice Structure Evolution during Phase Transformation of Zr-2.5Nb, Adv. Eng. Mater. 13(9), 882-886 (2011) (from ECHIDNA, WOMBAT)

145. Yan, T; Zheng, FF; Yu, YG; Qin, SB; Liu, H; Wang, JY and Yu, DH, Formation mechanism of black $LiTaO_3$ single crystals through chemical reduction, J. Appl. Crystallogr. 44, 158-162 (2011)

146. Yang, XS; Yuan, LX; Peterson, VK; Yin, YB; Minett, AI and Harris, AT, Open-Ended Aligned Carbon Nanotube Arrays Produced Using CO_2-Assisted Floating-Ferrocene Chemical Vapor Deposition, J. Phys. Chem. C 115(29), 14093-14097 (2011)

147. Yang, ZX; Du, GD; Guo, ZP; Yu, XB; Chen, ZX; Guo, TL; Sharma, N and Liu, HK, TiO_2(B)-anatase hybrid nanowires with highly reversible electrochemical performance, Electrochem. Commun. 13(1), 46-49 (2011)

148. Yao, SH; Wang, JY; Liu, H; Yan, T; Yu, DH and Chen, YF, Mechanism of the abnormal thermal expansion of nearly stoichiometric $LiNbO_3$, J. Cryst. Growth 318(1), 951-953 (2011)

149. Yaron, PN; Scott, AJ; Reynolds, PA; Mata, JP and White, JW, High Internal Phase Emulsions under Shear. Co-Surfactancy and Shear Stability, J. Phys. Chem. B 115(19), 5775-5784 (2011)

150. Zeng, R; Debnath, JC; Chen, DP; Shamba, P; Wang, JL; Kennedy, SJ; Campbell, SJ; Silver, T and Dou, SX, Magnetic properties in polycrystalline and single crystal Ca-doped $LaCoO_3$, J. Appl. Phys. 109(7), Art. No. 07E146 (2011)

151. Zeng, R; Dou, SX; Wang, JL and Campbell, SJ, Large magnetocaloric effect in re-entrant ferromagnet $PrMn_{1.4}Fe_{0.6}Ge_2$, J. Alloy. Compd. 509(7), L119-L123 (2011)

152. Zhang, J; Kisi, EH and Kirstein, O, Quantitative Neutron Diffraction Texture Measurement Applied to α-phase Alumina and Ti_3AlC_2, J. Appl. Crystallogr. 44(5), 1062-1070 (2011) (from KOWARI)

153. Zhao, M; Yang, X; Church, TL and Harris, AT, Interaction between a bimetallic Ni-Co catalyst and micrometer-sized CaO for enhanced H_2 production during cellulose decomposition, Int. J. Hydrogen Energy 36(1), 421-431 (2011)

154. Zhou, QD; Kennedy, BJ and Avdeev, M, Thermal expansion behaviour in the oxygen deficient perovskites $Sr_2BSbO_{5.5}$ B=Ca, Sr, Ba. Competing effects of water and oxygen ordering., J. Solid State Chem. 184(9), 2559-2565 (2011) (from ECHIDNA)

155. del Rio, MS; Garcia-Romero, E; Suarez, M; da Silva, I; Fuentes-Montero, L and Martinez-Criado, G, Variability in sepiolite: Diffraction studies, Am. Mineral. 96(10), 1443-1454 (2011)

2012

1. Ahmed, R; Faisal, N; Paradowska, A and Fitzpatrick, M, Residual Strain and Fracture Response of Al_2O_3 Coatings Deposited via APS and HVOF Techniques, Journal of Thermal Spray Technology 21(1), 23-40 (2012)

2. Aravind, N; Sissons, M; Egan, N; Fellows, CM; Blazek, J and Gilbert, EP, Effect of beta-Glucan on Technological, Sensory, and Structural Properties of Durum Wheat Pasta, Cereal Chemistry 89(2), 84-93 (2012) (from Bruker (SAXS))

3. Aravind, N; Sissons, MJ; Fellows, CM; Blazek, J and Gilbert, EP, Effect of inulin soluble dietary fibre addition on technological, sensory, and structural properties of durum wheat spaghetti, Food Chem. 132(2), 993-1002 (2012)

4. Auckett, JE; Studer, AJ; Sharma, N and Ling, CD, Floating-zone growth of brownmillerite $Sr_2Fe_2O_5$ and the observation of a chain-ordered superstructure by single-crystal neutron diffraction, Solid State Ionics 225, 432-436 (2012) (from WOMBAT)

5. Avdeev, M; Sale, M; Adams, S and Rao, RP, Screening of the alkali-metal ion containing materials from the Inorganic Crystal Structure Database (ICSD) for high ionic conductivity pathways using the bond valence method, Solid State Ionics 225, 43-46 (2012) (from Computing Cluster)

6. Baczmanski, A; Gaj, A; Le Joncour, L; Wronski, S; Francois, M; Panicaud, B; Braham, C and Paradowska, AM, Study of stress localisation in polycrystalline grains using self-consistent modelling and neutron diffraction, Philosophical Magazine 92(24), 3015-3035 (2012)

7. Baikie, T; Schreyer, MK; Wong, CL; Pramana, SS; Klooster, WT; Ferraris, C; McIntyre, GJ and White, TJ, A multi-domain gem-grade Brazilian apatite, Am. Mineral. 97(10), 1574-1581 (2012)

8. Barpanda, P; Avdeev, M; Ling, CD; Lu, J and Yamada, A, Magnetic Structure and Properties of the $Na_2CoP_2O_7$ Pyrophosphate Cathode for Sodium-Ion Batteries: A Supersuperexchange-Driven Non-Collinear Antiferromagnet, Inorg. Chem. 52, 395-401 (2012) (from ECHIDNA)

9. Barraud, N; Kardak, BG; Yepuri, NR; Howlin, RP; Webb, JS; Faust, SN; Kjelleberg, S; Rice, SA and Kelso, MJ, Cephalosporin-3'-diazeniumdiolates: Targeted NO-Donor Prodrugs for Dispersing Bacterial Biofilms, Angew. Chem. Int. Ed. Engl. 51(36), 9057-9060 (2012)

10. Bartkowiak, M; Mulders, AM; Scagnoli, V; Staub, U; Pomjakushina, E and Conder, K, Evolution of charge order through the magnetic phase transition of $LuFe_2O_4$, Physical Review B 86, Art. No. 035121 (2012)

11. Baszczuk, A; Dabrowski, B; Kolesnik, S; Chmaissem, O and Avdeev, M, Structural and physical properties of Re substituted B-site ordered and disordered $SrCo_{1-x}Re_xO_{3-\delta}$ (x=0.1, 0.25, 0.5), J. Solid State Chem. 186, 240-246 (2012) (from ECHIDNA)

12. Beale, TAW; Beutier, G; Bland, SR; Bombardi, A; Bouchenoire, L; Bunau, O; Di Matteo, S; Fernandez-Rodriguez, J; Hamann-Borrero, JE; Herrero-Martin, J; Jacques, VLR; Johnson, RD; Juhin, A; Matsumura, T; Mazzoli, C; Mulders, AM; Nakao, H; Okamoto, J; Partzsch, S; Princep, AJ; Scagnoli, V; Strempfer, J; Vecchini, C; Wakabayashi, Y; Walker, HC; Wermeille, D and Yamasaki, Y, REXS contribution to electronic ordering investigation in solids, Eur. Phys. J. Spec. Top. 208(1), 89-98 (2012)

13. Bentley, PM; Kennedy, SJ; Andersen, KH; Rodriguez, DM and Mildner, DFR, Correction of optical aberrations in elliptic neutron guides, Nucl. Instrum. Methods Phys. Res., Sect. A 693, 268-275 (2012)

14. Bhati, M; Lee, C; Gadd, MS; Jeffries, CM; Kwan, A; Whitten, AE; Trewhella, J; Mackay, JP and Matthews, JM, Solution Structure of the LIM-Homeodomain Transcription Factor Complex Lhx3/Ldb1 and the Effects of a Pituitary Mutation on Key Lhx3 Interactions, PLoS ONE 7(7), Art. No. e40719 (2012)

15. Blanchard, PER; Clements, R; Kennedy, BJ; Ling, CD; Reynolds, E; Avdeev, M; Stampfl, APJ; Zhang, Z and Jang, L-Y, Does Local Disorder Occur in the Pyrochlore Zirconates?, Inorg. Chem. 51, 13237-13244 (2012) (from ECHIDNA)

16. Bloch, ED; Queen, WL; Krishna, R; Zadrozny, JM; Brown, CM and Long, JR, Hydrocarbon Separations in a Metal-Organic Framework with Open Iron(II) Coordination Sites, Science 335(6076), 1606-1610 (2012) (from ECHIDNA)

17. Boekelheide, Z; Saerbeck, T; Stampfl, APJ; Robinson, RA; Stewart, DA and Hellman, F, Antiferromagnetism in Cr_3Al and relation to semiconducting behavior, Phys. Rev. B: Condens. Matter Mater. Phys. 85(9), Art. No. 094413 (2012) (from TAIPAN)

18. Bongiovanni, R; Nelson, A; Vitale, A and Bernardi, E, Ultra-thin films based on random copolymers containing perfluoropolyether side chains, Thin Solid Films 520(17), 5627-5632 (2012) (from X-ray reflectometer)

19. Bot, A; Gilbert, EP; Bouwman, WG; Sawalha, H; den Adel, R; Garamus, VM; Venema, P; van der Linden, E and Floter, E, Elucidation of density profile of self-assembled sitosterol + oryzanol tubules with small-angle neutron scattering, Faraday Discuss. 158, 223-238 (2012) (from QUOKKA)

20. Brant, WR; Schmid, S; Kuhn, A; Hester, J; Avdeev, M; Sale, M and Gu, Q, Rapid Lithium Insertion and Location of Mobile Lithium in the Defect Perovskite $Li_{0.18}Sr_{0.66}Ti_{0.5}Nb_{0.5}O_3$, ChemPhysChem 13(9), 2293-2296 (2012) (from ECHIDNA)

21. Cadogan, JM; Lemoine, P; Slater, BR; Mar, A and Avdeev, M, Neutron Diffraction Study of the Hexagonal Perovskite-Type Compound $LaCrGe_3$, Solid. State Phenom. 194, 71-74 (2012) (from ECHIDNA)

22. Chantler, CT; Rae, NA; Islam, MT; Best, SP; Yeo, J; Smale, LF; Hester, J; Mohammadi, N and Wang, F, Stereochemical analysis of ferrocene and the uncertainty of fluorescence XAFS data, Journal of Synchrotron Radiation 19, 145-158 (2012)

23. Chen, X; Wilde, KL; Wang, H; Lake, V; Holden, PJ; Middelberg, APJ; He, L and Duff, AP, High yield expression and efficient purification of deuterated human protein galectin-2, Food and Bioproducts Processing 90(3), 563-572 (2012) (from NDF - Biodeuteration)

24. Chiang, CY; Su, HC; Wu, PJ; Liu, HJ; Hu, CW; Sharma, N; Peterson, VK; Hsieh, HW; Lin, YF; Chou, WC; Lee, CH; Lee, JF and Shew, BY, Vanadium Substitution of $LiFePO_4$ Cathode Materials To Enhance the Capacity of $LiFePO_4$-Based Lithium-Ion Batteries, J. Phys. Chem. C 116, 24424-24429 (2012) (from ECHIDNA)

25. Choucair, M and Stride, JA, The gram-scale synthesis of carbon onions, Carbon 50(3), 1109-1115 (2012)

26. Choucair, M; Gong, B and Stride, JA, Engineering solvothermal reactions to produce multi-walled carbon nanotubes, Journal of Nanoparticle Research 14(6), Art. No. 901 (2012)

27. Choucair, M; Tse, NMK; Hill, MR and Stride, JA, Adsorption and desorption characteristics of 3-dimensional networks of fused graphene, Surface Science 606(1-2), 34-39 (2012)

28. Christie, MP; Whitten, AE; King, GJ; Hu, SH; Jarrott, RJ; Chen, KE; Duff, AP; Callow, P; Collins, BM; James, DE and Martin, JL, Low-resolution solution structures of Munc18:Syntaxin protein complexes indicate an open binding mode driven by the Syntaxin N-peptide, Proceedings of the National Academy of Sciences of the United States of America 109(25), 9816-9821 (2012) (from NDF - Biodeuteration)

29. Ciampi, S; James, M; Le Saux, G; Gaus, K and Justin Gooding, J, Electrochemical 'Switching' of Silicon(100) Modular Assemblies, J. Am. Chem. Soc. 134(2), 844-847 (2012) (from X-ray reflectometer)

30. Clifton, LA; Johnson, CL; Solovyova, AS; Callow, P; Weiss, KL; Ridley, H; Le Brun, AP; Kinane, CJ; Webster, JRP; Holt, SA and Lakey, JH, Low Resolution Structure and Dynamics of a Colicin-Receptor Complex Determined by Neutron Scattering, J. Biol. Chem. 287(1), 337-346 (2012)

31. Cortie, DL and Lewis, RA, The importance of scattering, surface potential, and vanguard counter-potential in terahertz emission from gallium arsenide, Appl. Phys. Lett. 100(26), Art. No. 61601 (2012)

32. Cortie, DL; Lin, KW; Shueh, C; Hsu, HF; Wang, XL; James, M; Fritzsche, H; Brück, S and Klose, F, Exchange bias in a nanocrystalline hematite/permalloy thin film investigated with polarized neutron reflectometry, Physical Review B 86(5), Art. No. 054408 (2012) (from PLATYPUS)

33. Cortie, DL; Shueh, C; Chen, PS; Gao, JF; Klose, F; van Lierop, J and Lin, KW, Probing Exchange Bias Effects in CoO/Co Bilayers with Pillar-Like CoO Structures, Jpn. J. Appl. Phys. 51, Art. No. PG101 (2012)

34. Cortie, DL; Stampfl, APJ; Klose, F; Du, Y; Wang, XL; Zhao, HY; Kimura, H and Cheng, ZX, The magnetic structure of an epitaxial $BiMn_{0.5}Fe_{0.5}O_3$ thin film on $SrTiO_3$ (001) studied with neutron diffraction, Appl. Phys. Lett. 101, Art. No. 72404 (2012) (from TAIPAN)

35. Danilkin, SA; Avdeev, M; Sale, M and Sakuma, T , Neutron scattering study of ionic diffusion in Cu-Se superionic compounds, Solid State Ionics 225, 190-193 (2012) (from ECHIDNA)

36. Danilkin, SA; Yethiraj, M; Saerbeck, T; Klose, F; Ulrich, C; Fujioka, J; Miyasaka, S; Tokura, Y and Keimer, B, TAIPAN: First Results from the Thermal Triple-axis Spectrometer at OPAL Research Reactor, J. Phys.: Conf. Ser. 340(1), Art. No. 012003 (2012) (from TAIPAN)

37. Darwish, TA; Smith, ARG; Gentle, IR; Burn, PL; Luks, E; Moraes, G; Gillon, M; Holden, PJ and James, M, Deuteration of molecules for neutron reflectometry on organic light-emitting diode thin films, Tetrahedron Letters 53(8), 931-935 (2012) (from NDF - Chemical Deuteration, PLATYPUS)

38. Darwish, TA; Tong, Y; James, M; Hanley, TL; Peng, Q and Ye, S, Characterizing the Photoinduced Switching Process of a Nitrospiropyran Self-Assembled Monolayer Using In Situ Sum Frequency Generation Spectroscopy, Langmuir 28(39), 13852-13860 (2012) (from NDF - Chemical Deuteration)

39. Deng, G; Thiyagarajan, R; Mohan Radheep, D; Pomjakushina, E; Medarde, M; Krzton-Maziopa, A; Wang, S; Arumugam, S and Conder, K , Floating zone crystal growth and magnetic properties of bilayer manganites $Pr(Sr_{1-x}Ca_x)_2Mn_2O_7$, J. Cryst. Growth 353(1), 25-30 (2012)

40. Diao, H; Yan, C; Bell, JM; Lu, L; Zhang, GP; Kabra, S; Liss, KD and Chen, MW, Compressive behaviour of nanocrystalline Mg-5Al alloys, Materials Technology: Advanced Performance Materials 27(1), 85-87 (2012) (from WOMBAT)

41. Dimitrijev-Dwyer, M; He, L; James, M; Nelson, A; Wang, L and Middelberg, APJ, The effects of acid hydrolysis on protein biosurfactant molecular, interfacial, and foam properties: pH responsive protein hydrolysates, Soft Matter 8(19), 5131-5139 (2012) (from NDF - Biodeuteration, PLATYPUS)

42. Dissanayake, SE; Chan, C; Ji, S; Lee, J; Qiu, Y; Rule, KC; Lake, B; Green, M; Hagihala, M; Zheng, XG; Ng, TK and Lee, SH, Magnetic-field-induced instability of the cooperative paramagnetic state in $Zn_xCo_{(4-x)}(OD)_6C_{l2}$, Physical Review B 85(17), Art. No. 174435 (2012)

43. Doutch, J; Bason, M; Franceschini, F; James, K; Clowes, D and Gilbert, EP, Structural changes during starch pasting using simultaneous Rapid Visco Analysis and small-angle neutron scattering, Carbohydr. Polym. 88(3), 1061-1071 (2012) (from QUOKKA)

44. Doutch, J; Hough, MA; Hasnain, SS and Strange, RW, Challenges of sulfur SAD phasing as a routine method in macromolecular crystallography, J. Synchrot. Radiat. 19, 19-29 (2012)

45. Doutch, JJ; Quantock, AJ; Joyce, NC and Meek, KM, Ultraviolet Light Transmission through the Human Corneal Stroma Is Reduced in the Periphery, Biophys. J. 102(6), 1258-1264 (2012)

46. Driza, N; Blanco-Canosa, S; Bakr, M; Soltan, S; Khalid, M; Mustafa, L; Kawashima, K; Christiani, G; Habermeier, HU; Khaliullin, G; Ulrich, C; Le Tacon, M and Keimer, B, Long-range transfer of electron-phonon coupling in oxide superlattices, Nat. Mater. 11(8), 675-681 (2012)

47. Du, F; Ohgushi, K; Nambu, Y; Kawakami, T; Avdeev, M; Hirata, Y; Watanabe, Y; Sato, TJ and Ueda, Y, Stripelike magnetism in a mixed-valence insulating state of the Fe-based ladder compound CsF_2Se_3, Phys. Rev. B: Condens. Matter Mater. Phys. 85(21), Art. No. 214436 (2012) (from ECHIDNA)

48. Duffort, V; Caignaert, V; Pralong, V; Barrier, N; Raveau, B; Avdeev, M; Zheng, H and Mitchell, JF, Tetragonal $YBaFe_4O_{7.0}$: A stoichiometric polymorph of the "114" ferrite family, J. Solid State Chem. 191, 225-231 (2012) (from ECHIDNA)

49. Dung, NH; Zhang, L; Ou, ZQ; Zhao, L; van Eijck, L; Mulders, AM; Avdeev, M; Suard, E; van Dijk, NH and Brück, E, High/low-moment phase transition in hexagonal Mn-Fe-P-Si compounds, Physical Review B 86(4), Art. No. 045134 (2012) (from ECHIDNA)

50. Ener, S; Neuhaus, J; Petry, W; Mole, R; Hradil, K; Siewert, M; Gruner, ME; Entel, P; Titov, I and Acet, M, Effect of temperature and compositional changes on the phonon properties of Ni-Mn-Ga shape memory alloys, Phys. Rev. B 86(14), Art. No. 4305 (2012)

51. Ehlers, G; Huq, A; Diallo, SO; Adriano, C; Rule, KC; Cornelius, AL; Fouquet, P; Pagliuso, PG and Gardner, JS, Low energy spin dynamics in the spin ice $Ho_2Sn_2O_7$, J. Phys.: Condens. Matter 24(7), Art. No. 076005 (2012)

52. Fernandez, DI; Le Brun, AP; Whitwell, TC; Sani, M-A; James, M and Separovic, F, The antimicrobial peptide aurein 1.2 disrupts model membranes via the carpet mechanism, Phys. Chem. Chem. Phys. 14(45), 15739-15751 (2012) (from PLATYPUS)

53. Fucke, K; McIntyre, GJ; Wilkinson, C; Henry, M; Howard, JAK and Steed, JW, New Insights into an Old Molecule: Interaction Energies of Theophylline Crystal Forms, Cryst. Growth Des 12(3), 1395-1401 (2012)

54. Gallat, FX; Laganowsky, A; Wood, K; Gabel, F; van Eijck, L; Wuttke, J; Moulin, M; Hartlein, M; Eisenberg, D; Colletier, JP; Zaccai, G and Weik, M, Dynamical Coupling of Intrinsically Disordered Proteins and Their Hydration Water: Comparison with Folded Soluble and Membrane Proteins, Biophys. J. 103(1), 129-136 (2012)

55. Gatta, GD; McIntyre, GJ; Bromiley, G; Guastoni, A and Nestola, F, A single-crystal neutron diffraction study of hambergite, $Be_2BO_3(OH,F)$, Am. Mineral. 97(11-12), 1891-1897 (2012) (from Koala)

56. Gatta, GD; McIntyre, GJ; Swanson, JG and Jacobsen, SD, Minerals in cement chemistry: A single-crystal neutron diffraction and Raman spectroscopic study of thaumasite, $Ca_3Si(OH)_6(CO_3)(SO_4)\cdot 12H_2O$, Am. Mineral. 97(7), 1060-1069 (2012)

57. Geiger, CA; Gatta, GD; Xue, X and McIntyre, GJ, A neutron/X-Ray diffraction, IR, and $^1H/^{29}Si$ NMR Spectroscopic investigation of armenite: behavior of extra framework Ca cations and H_2O molecules in microporous silicates, Zeitschrift Fur Kristallographie 227(7), 411-426 (2012)

58. Gerth, S; Klimczak, M; Nelson, A and Magerl, A, Near Surface Crystallization of Pluronic P123, J. Phys.: Conf. Ser. 340(1), Art. No. 012088 (2012) (from PLATYPUS)

59. Goossens, DJ; Henderson, LSF; Trevena, S; Hudspeth, JM; Avdeev, M and Hester, JR, The crystal and magnetic structures of $LaCa_2Fe_{3-x}M_xO_8$ (M=Al, Ga, In), J. Solid State Chem. 196, 238-242 (2012) (from ECHIDNA)

60. Goossens, DJ; Whitfield, RE and Studer, AJ, Optimising Sintering in Metal Injection Moulding Using In Situ Neutron Diffraction, Mater. Sci. Forum 706-709, 1737-1742 (2012) (from WOMBAT)

61. Grant, DJ; Stewart, TJ; Bau, R; Miller, KA; Mason, SA; Gutmann, M; McIntyre, GJ; Gagliardi, L and Evans, WJ, Uranium and Thorium Hydride Complexes as Multielectron Reductants: A Combined Neutron Diffraction and Quantum Chemical Study, Inorg. Chem. 51(6), 3613-3624 (2012)

62. Guan, B; Ciampi, S; Luais, E; James, M; Reece, PJ and Gooding, JJ, Depth-Resolved Chemical Modification of Porous Silicon by Wavelength-Tuned Irradiation, Langmuir 28(44), 15444-15449 (2012) (from X-ray reflectometer)

63. Gummow, RJ; Sharma, N; Peterson, VK and He, Y, Crystal chemistry of the Pmnb polymorph of Li_2MnSiO_4, J. Solid State Chem. 188, 32-37 (2012) (from ECHIDNA)

64. Haque, R; Beynon, JH; Durandet, Y; Kirstein, O and Blacket, S, Feasibility of measuring residual stress profile in different Self-Pierce Riveted joints , Sci. Technol. Weld. Joi. 17(1), 60-68 (2012) (from KOWARI)

65. Haque, R; Beynon, JH; Kirstein, O; Wong, YC and Durandet, Y, Evaluation of Residual Stress in SPR Joint by Neutron Diffraction, Adv. Mater. Res. 409, 575-580 (2012) (from KOWARI)

66. Haverkate, LA; Zbiri, M; Johnson, MR; Deme, B; de Groot, HJM; Lefeber, F; Kotlewski, A; Picken, SJ; Mulder, FM and Kearley, GJ, On the Morphology of a Discotic Liquid Crystalline Charge Transfer Complex, J. Phys. Chem. B 116(43), 13098-13105 (2012) (from Computing Cluster)

67. Hong, D; Shin, K; James, M and Tae, G, Mimicking the receptor-aided binding of HIV-1 TAT protein transduction domains to phospholipid monolayers at the air-water interface, Soft Matter 8(33), 8616-8623 (2012) (from X-ray reflectometer)

68. Hsu, Y-C; Weir, MP; Truss, RW; Garvey, CJ; Nicholson, TM and Halley, PJ, A fundamental study on photo-oxidative degradation of linear low density polyethylene films at embrittlement, Polymer 53(12), 2385-2393 (2012)

69. Hudson, MR; Queen, WL; Mason, JA; Fickel, DW; Lobo, RF and Brown, CM, Unconventional and Highly Selective CO_2 Adsorption in Zeolite SSZ-13, J. Am. Chem. Soc. 134(4), 1970-1973 (2012) (from ECHIDNA)

70. Huh, M; Jung, M-H; Park, YS; Kang, T-B; Nah, C; Russell, RA; Holden, PJ and Yun, SI, Fabrication of honeycomb-structured porous films from poly(3-hydroxybutyrate) and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) via the breath figures method, Polymer Engineering & Science 52(4), 920-926 (2012)

71. Hutchison, WD; Goossens, DJ; Whitfield, RE; Studer, AJ; Nishimura, K and Mizushima, T, Field-induced incommensurate spin structure of $TbNiAl_4$, Physical Review B 86, Art. No. 014412 (2012) (from WOMBAT)

72. Hynson, RMG; Jeffries, CM; Trewhella, J and Cocklin, S, Solution structure studies of monomeric human TIP47/perilipin-3 reveal a highly extended conformation, Proteins-Structure Function and Bioinformatics 80(8), 2046-2055 (2012)

73. Jones, AOF; Lemee-Cailleau, M-H; Martins, DMS; McIntyre, GJ; Oswald, IDH; Pulham, CR; Spanswick, CK; Thomas, LH and Wilson, CC , Temperature dependent solid-state proton migration in dimethylurea-oxalic acid complexes, Phys. Chem. Chem. Phys. 14(38), 13273-13283 (2012)

74. Jones, JL; Aksel, E; Tutuncu, G; Usher, TM; Chen, J; Xing, XR and Studer, AJ, Domain wall and interphase boundary motion in a two-phase morphotropic phase boundary ferroelectric: Frequency dispersion and contribution to piezoelectric and dielectric properties, Physical Review B 86(2), Art. No. 4104 (2012) (from WOMBAT)

75. Juarez-Arellano, EA; Avdeev, M; Yakovlev, S; Lopez-de-la-Torre, L; Bayarjargal, L; Winkler, B; Friedrich, A and Kharton, VV, High-pressure behavior and equations of state of the cobaltates and $YBaCo_4O_{7+\delta}$, $YBaCo_4O_{7+\delta}$, $YBaCoZn_3O_7$ and $BaCoO_{3-x}$, J. Solid State Chem. 196, 209-216 (2012) (from ECHIDNA)

76. Kandemir, T; Girgsdies, F; Kasatkin, I; Kunkes, E; Liss, K-D; Peterson, VK; Schlögl, R and Behrens, M, Heterogeneous Catalysis under pressure - In-situ neutron diffraction under industrial conditions, J. Phys.: Conf. Ser. 340(1), Art. No. 012053 (2012) (from ECHIDNA)

77. Kandemir, T; Wallacher, D; Hansen, T; Liss, K-D; Naumann d'Alnoncourt, R; Schlögl, R and Behrens, M, In situ neutron diffraction under high pressure - Providing an insight into working catalysts, Nucl. Instrum. Methods Phys. Res., Sect. A 673, 51-55 (2012) (from ECHIDNA)

78. Kaneko, F; Sasaki, K; Kawaguchi, T; Ute, K and Hester, J, Neutron Diffraction and IR Spectroscopy Study on Crystalline Complexation of Syndiotactic Polystyrene with 15-Crown-5 and 18-Crown-6, Chemistry Letters 41(3), 284-286 (2012) (from ECHIDNA)

79. Kearley, GJ; Stare, J; Kutteh, R; Daemen, LL; Hartl, MA and Eckert, J, Methyl Dynamics Flattens Barrier to Proton Transfer in Crystalline Tetraacetylethane, Journal of Physical Chemistry A 116(9), 2283-2291 (2012) (from Computing Cluster)

80. Kennaway, CK; Taylor, JE; Song, CF; Potrzebowski, W; Nicholson, W; White, JH; Swiderska, A; Obarska-Kosinska, A; Callow, P; Cooper, LP; Roberts, GA; Artero, J-B; Bujnicki, JM; Trinick, J; Kneale, GG and Dryden, DTF, Structure and operation of the DNA-translocating type I DNA restriction enzymes, Genes & Development 26(1), 92-104 (2012) (from Bruker (SAXS))

81. Knupfer, SM; Paradowska, AM; Kirstein, O and Moore, AJ, Characterization of the residual strains in iterative laser forming, J. Mater. Process. Tech. 212(1), 90-99 (2012) (from KOWARI)

82. Kolesnik, S; Dabrowski, B; Chmaissem, O; Avci, S; Hodges, JP; Avdeev, M and Swierczek, K, Enhancement of the Curie temperature in $NdBaCo_2O_{5.5}$ by A-site Ca substitution , Physical Review B 86(6), Art. No. 064434 (2012) (from ECHIDNA)

83. Lauw, Y; Horne, MD; Rodopoulos, T; Lockett, V; Akgun, B; Hamilton, WA and Nelson, ARJ, Structure of [C4mpyr][NTf2] Room-Temperature Ionic Liquid at Charged Gold Interfaces, Langmuir 28(19), 7374-738 (2012) (from Computing Cluster, PLATYPUS, X-ray reflectometer)

84. Law, M and Luzin, V, Measured residual stresses and integrity of pipeline girth welds, Sci. Technol. Weld. Joi. 17(8), 694-698 (2012) (from KOWARI)

85. Law, M; Kirstein, O and Luzin, V, Effect of residual stress on the integrity of a branch connection, International Journal of Pressure Vessels and Piping 96-97, 24-29 (2012) (from KOWARI)

86. Le Brun, AP; Chow, J; Bax, DV; Nelson, A; Weiss, AS and James, M, Molecular Orientation of Tropoelastin is Determined by Surface Hydrophobicity, Biomacromolecules 13(2), 379-386 (2012) (from PLATYPUS)

87. Lee, E; Park, C-H; Shoemaker, DP; Avdeev, M and Kim, Y-I, Crystal structure analysis of tungsten bronzes β-$SrTa_2O_6$ and β'-$SrTa_2O_6$ by synchrotron X-ray and neutron powder diffraction, J. Solid State Chem. 191, 232-238 (2012) (from ECHIDNA)

88. Li, D; Huang, YD; Sharma, N; Chen, ZX; Jia, DZ and Guo, ZP, Enhanced electrochemical properties of $LiFePO_4$ by Mo-substitution and graphitic carbon-coating via a facile and fast microwave-assisted solid-state reaction, Phys. Chem. Chem. Phys. 14(10), 3634-3639 (2012)

89. Li, HA; Baikie, T; Pramana, SS; Shin, JF; Slater, PR; Brink, F; Hester, J; Wallwork, K and White, TJ, Synthesis and characterisation of vanadium doped alkaline earth lanthanum germanate oxyapatite electrolyte, J. Mater. Chem 22(6), 2658-2669 (2012) (from ECHIDNA)

90. Li, Q; Liu, Y; Luzin, V; Studer, AJ; Wan, Y; Li, Z; Noren, L; Withers, RL and Xu, Z, In-situ neutron diffraction study of $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ single crystals under uniaxial mechanical stress , J. Appl. Phys. 111(8), Art. No. 084110 (2012) (from KOWARI)

91. Li, Y; Yu, G; Chan, MK; Baledent, V; Barisic, N; Zhao, X; Hradil, K; Mole, RA; Sidis, Y; Steffens, P; Bourges, P and Greven, M, Two Ising-like magnetic excitations in a single-layer cuprate superconductor, Nature Physics 8(5), 404-410 (2012)

92. Liao, P-K; Fang, C-S; Edwards, AJ; Kahlal, S; Saillard, J-Y and Liu, CW, Hydrido Copper Clusters Supported by Dithiocarbamates: Oxidative Hydride Removal and Neutron Diffraction Analysis of $[Cu_7(H)\{S_2C(aza\text{-}15\text{-}crown\text{-}5)\}_6]$, Inorg. Chem. 51(12), 6577-6591 (2012) (from Koala)

93. Ling, CD; Miiler, W; Johnson, MR; Richard, D; Rols, S; Madge, J and Evans, IR, Local Structure, Dynamics, and the Mechanisms of Oxide Ionic Conduction in $Bi_{26}Mo_{10}O_{69}$, Chem. Mater. 24(23), 4607-4614 (2012)

94. Liu, FS; Romanova, N; Lee, EA; Ahmed, R; Evans, M; Gilbert, EP; Morell, MK; Emes, MJ and Tetlow, IJ, Glucan affinity of starch synthase IIa determines binding of starch synthase I and starch-branching enzyme IIb to starch granules, Biochem. J. 448, 373-387 (2012)

95. Liu, J; Toulouse, C; Rovillain, P; Cazayous, M; Gallais, Y; Measson, MA; Lee, N; Cheong, SW and Sacuto, A, Lattice and spin excitations in multiferroic h-$YbMnO_3$, Phys. Rev. B 86(18), Art. No. 184410 (2012)

96. Liu, Y; Norén, L; Studer, AJ; Withers, RL; Guo, Y; Li, Y; Yang, H and Wang, J, Response of intergrown microstructure to an electric field and its consequences in the lead-free piezoelectric bismuth sodium titanate, J. Solid State Chem. 187, 309-315 (2012) (from WOMBAT)

97. Low, HR; Avdeev, M; Ramesh, K and White, TJ , Zinc Hydroxyapatite Catalyst for Decomposition of 2-Propanol, Adv. Mater. 24(30), 4175-4179 (2012) (from ECHIDNA)

98. Lu, Y; Kwan, AH; Jeffries, CM; Guss, JM and Trewhella, J, The Motif of Human Cardiac Myosin-binding Protein C Is Required for Its Ca^{2+}-dependent Interaction with Calmodulin, J. Biol. Chem. 287(37), 31596-31607 (2012)

99. Luo, H; Yamani, Z; Chen, Y; Lu, X; Wang, M; Li, S; Maier, TA; Danilkin, S; Adroja, DT and Dai, P, Electron doping evolution of the anisotropic spin excitations in $BaFe_{(2-x)}Ni_xAs_2$, Physical Review B 86(2), Art. No. 024508 (2012) (from TAIPAN)

100. Menzies, DJ; Nelson, A; Shen, HH; McLean, KM; Forsythe, JS; Gengenbach, T; Fong, C and Muir, BW, An X-ray and neutron reflectometry study of 'PEG-like' plasma polymer films, J. R. Soc. Interface 9(70), 1008-1019 (2012) (from PLATYPUS, X-ray reflectometer)

101. Miiller, W; Auckett, J; Avdeev, M and Ling, CD, Coexistence of spin glass and antiferromagnetic orders in $Ba_3Fe_{2.15}W_{0.85}O_{8.72}$, J. Phys.: Condens. Matter 24(20), Art. No. 206004 (2012) (from Computing Cluster, ECHIDNA, Koala)

102. Miiller, W; Avdeev, M; Zhou, Q; Kennedy, BJ; Sharma, N; Kutteh, R; Kearley, GJ; Schmid, S; Knight, KS; Blanchard, PER and Ling, CD, Giant Magnetoelastic Effect at the Opening of a Spin-Gap in $Ba_3BiIr_2O_9$, J. Am. Chem. Soc. 134(6), 3265-3270 (2012) (from Computing Cluster, ECHIDNA)

103. Miiller, W; Kearley, G and Ling, C, Ab initio parametrized polarizable force field for rutile-type SnO_2, Theor. Chem. Acc. 131(5), Art. No. 1216 (2012) (from Computing Cluster)

104. Morris, VK; Linser, R; Wilde, KL; Duff, AP; Sunde, M and Kwan, AH, Solid-State NMR Spectroscopy of Functional Amyloid from a Fungal Hydrophobin: A Well-Ordered β-Sheet Core Amidst Structural Heterogeneity, Angew. Chem. Int. Ed. Engl. 51(50), 12621-12625 (2012) (from NDF - Biodeuteration)

105. Muransky, O; Smith, MC; Bendeich, PJ; Holden, TM; Luzin, V; Martins, RV and Edwards, L, Comprehensive numerical analysis of a three-pass bead-in-slot weld and its critical validation using neutron and synchrotron diffraction residual stress measurements, International Journal of Solids and Structures 49(9), 1045-1062 (2012) (from ECHIDNA, KOWARI)

106. Nambu, Y; Ohgushi, K; Suzuki, S; Du, F; Avdeev, M; Uwatoko, Y; Munakata, K; Fukazawa, H; Chi, S; Ueda, Y and Sato, TJ, Block magnetism coupled with local distortion in the iron-based spin-ladder compound $BaFe_2Se_3$, Phys. Rev. B: Condens. Matter Mater. Phys. 85, Art. No. 064413 (2012) (from ECHIDNA)

107. Ng, MCC; Harper, JB; Stampfl, APJ; Kearley, GJ; Rols, S and Stride, JA, Central-Atom Size Effects on the Methyl Torsions of Group XIV Tetratolyls, Chemistry-a European Journal 18(41), 13018-13024 (2012) (from Computing Cluster)

108. Omrani, AA; Deng, G; Radenovic, A; Kis, A and Ronnow, HM, Micro-fabrication process for small transport devices of layered manganite, J. Appl. Phys. 111(7), Art. No. 07E129 (2012)

109. Paddea, S; Francis, JA; Paradowska, AM; Bouchard, PJ and Shibli, IA, Residual stress distributions in a P91 steel-pipe girth weld before and after post weld heat treatment, Materials Science and Engineering: A 534, 663-672 (2012)

110. Pierret, S; Evans, A; Paradowska, AM; Kaestner, A; James, J; Etter, T and Van Swygenhoven, H, Combining neutron diffraction and imaging for residual strain measurements in a single crystal turbine blade, NDT & E International 45(1), 39-45 (2012)

111. Ping-Han Tsai, Mohammad H.N. Assadi, Tianshu Zhang, Clemens Ulrich, Thiam Teck Tan, Richard Donelson, and Sean Li, Immobilization of Na Ions for Substantial Power Factor Enhancement: Site-Specific Defect Engineering in $Na_{0.8}CoO_2$, J. Phys. Chem. C 116(6), 4324-4329 (2012)

112. Princep, AJ; Mulders, AM; Schierle, E; Weschke, E; Hester, J; Hutchison, WD; Tanaka, Y; Terada, N; Narumi, Y and Nakamura, T, High-order Ho multipoles in HoB_2C_2 observed with soft resonant x-ray diffraction, J. Phys.: Condens. Matter 24(7), Art. No. 075602 (2012) (from WOMBAT)

113. Queen, WL; Bloch, ED; Brown, CM; Hudson, MR; Mason, JA; Murray, LJ; Ramirez-Cuesta, AJ; Peterson, VK and Long, JR, Hydrogen Adsorption in the Metal-Organic Frameworks Fe_2(dobdc) and $Fe_2(O_2)$(dobdc), Dalton Trans. 41(14), 4180-4187 (2012) (from WOMBAT)

114. Quintero-Castro, DL; Lake, B; Islam, ATMN; Wheeler, EM; Balz, C; Månsson, M; Rule, KC; Gvasaliya, S and Zheludev, A, Asymmetric Thermal Line Shape Broadening in a Gapped 3D Antiferromagnet: Evidence for Strong Correlations at Finite Temperature, Phys. Rev. Lett. 109(12), Art. No. 127206 (2012)

115. Ravel, B; Hester, JR; Sole, VA and Newville, M, Towards data format standardization for X-ray absorption spectroscopy, J. Synchrot. Radiat. 19, 869-874 (2012)

116. Rayavarapu, PR; Sharma, N; Peterson, VK and Adams, S, Variation in structure and Li+-ion migration in argyrodite-type Li_6PS_5X (X = Cl, Br, I) solid electrolytes, Journal of Solid State Electrochemistry 16(5), 1807-1813 (2012) (from ECHIDNA)

117. Reehuis, M; Ulrich, C; Maljuk, A; Niedermayer, C; Ouladdiaf, B; Hoser, A; Hofmann, T and Keimer, B, Neutron diffraction study of spin and charge ordering in $SrFeO_{3-d}$, Physical Review B 85(18), Art. No. 184109 (2012)

118. Regina, A; Blazek, J; Gilbert, E; Flanagan, BM; Gidley, MJ; Cavanagh, C; Ral, J-P; Larroque, O; Bird, AR; Li, Z and Morell, MK, Differential effects of genetically distinct mechanisms of elevating amylose on barley starch characteristics, Carbohydr. Polym. 89(3), 979-991 (2012) (from Bruker (SAXS))

119. Rekas, A; Ahn, KJ; Kim, J and Carver, JA, The chaperone activity of a-synuclein: Utilizing deletion mutants to map its interaction with target proteins, Proteins-Structure Function and Bioinformatics 80(5), 1316-1325 (2012)

120. Robinson, JS; Tanner, DA; Truman, CE; Paradowska, AM and Wimpory, RC, The influence of quench sensitivity on residual stresses in the aluminium alloys 7010 and 7075, Materials Characterization 65, 73-85 (2012)

121. Rolph, J; Evans, A; Paradowska, A; Hofmann, M; Hardy, M and Preuss, M, Stress relaxation through ageing heat treatment – a comparison between in situ and ex situ neutron diffraction techniques, Comptes Rendus Physique 13(3), 307-315 (2012)

122. Rotundu, CR; Tian, W; Rule, KC; Forrest, TR; Zhao, J; Zarestky, JL and Birgeneau, RJ, Neutron scattering study of underdoped $Ba_{(1-x)}K_xFe_2As_2$ (x=0.09 and 0.17) self-flux-grown single crystals and the universality of the tricritical point , Physical Review B 85(14), Art. No. 144506 (2012)

123. Rovillain, P; Liu, J; Cazayous, M; Gallais, Y; Measson, MA; Sakata, H and Sacuto, A, Electromagnon and phonon excitations in multiferroic $TbMnO_3$, Phys. Rev. B 86(1), Art. No. 014437 (2012)

124. Saerbeck, T; Klose, F; Le Brun, AP; Fuzi, J; Brule, A; Nelson, A; Holt, SA and James, M, Polarization “Down Under”: The polarized time-of-flight neutron reflectometer PLATYPUS, Rev. Sci. Instrum. 83(8), Art. No. 081301 (2012)

125. Saerbeck, T; Loh, N; Lott, D; Toperverg, BP; Mulders, AM; Ali, M; Hickey, BJ; Stampfl, APJ; Klose, F and Stamps, RL, Specular and off-specular polarized neutron reflectometry of canted magnetic domains in loose spin coupled CuMn/Co multilayers, Phys. Rev. B: Condens. Matter Mater. Phys. 85(1), Art. No. 014411 (2012)

126. Sakaguchi, T; Kobayashi, Y; Yajima, T; Ohkura, M; Tassel, C; Takeiri, F; Mitsuoka, S; Ohkubo, H; Yamamoto, T; Kim, Je; Tsuji, N; Fujihara, A; Matsushita, Y; Hester, J; Avdeev, M; Ohoyama, K and Kageyama, H, Oxyhydrides of (Ca,Sr,Ba) TiO_3 Perovskite Solid Solutions, Inorg. Chem. 51(21), 11371-11376 (2012) (from ECHIDNA)

127. Sale, M and Avdeev, M, 3DBVSMAPPER: a program for automatically generating bond-valence sum landscapes, J. Appl. Crystallogr. 45, 1054-1056 (2012) (from Computing Cluster)

128. Samuel Yu Him Liu , Wojciech Miiller , Yun Liu , Max Avdeev , and Chris D. Ling, Sillen-Aurivillius Intergrowth Phases as Templates for Naturally Layered Multiferroics, Chem. Mater. 24(20), 3932-3942 (2012) (from ECHIDNA)

129. Sang, Y; Yu, D; Avdeev, M; Piltz, R; Sharma, N; Ye, N; Liu, H and Wang, J, X-ray and neutron diffraction studies of flux and hydrothermally grown nonlinear optical material $KBe_2BO_3F_2$, CrystEngComm 14(18), 6079-6084 (2012) (from ECHIDNA, Koala)

130. Sang, Y; Yu, D; Avdeev, M; Qin, H; Wang, J; Liu, H and Lv, Y, Yttrium aluminum garnet Nanoparticles with low antisite Defects studied with neutron and X-ray diffraction, J. Solid State Chem. 192, 366-370 (2012) (from ECHIDNA)

131. Satapathy, DK; Uribe-Laverde, MA; Marozau, I; Malik, VK; Das, S; Wagner, T; Marcelot, C; Stahn, J; Bruck, S; Ruhm, A; Macke, S; Tietze, T; Goering, E; Frano, A; Kim, JH; Wu, M; Benckiser, E; Keimer, B; Devishvili, A; Toperverg, BP; Merz, M; Nagel, P; Schuppler, S and Bernhard, C, Magnetic Proximity Effect in $YBa_2Cu_3O_7$/ $La_{(2/3)}Ca_{(1/3)}MnO_3$ and $YBa_2Cu_3O_7$/ $LaMnO_{(3+delta)}$ Superlattices, Phys. Rev. Lett. 108(19), Art. No. 197201 (2012)

132. Schmid, S and Fung, V, Incommensurate Modulated Structures in the $Ta_2O_5.Al_2O_3$ System, Aus. J. Chem. 65(7), 851-859 (2012) (from ECHIDNA)

133. Sharma, N and Peterson, VK, In situ neutron powder diffraction studies of lithium-ion batteries, Journal of Solid State Electrochemistry 16(5), 1849-1856 (2012) (from WOMBAT)

134. Sharma, N; Guo, XW; Du, GD; Guo, ZP; Wang, JZ; Wang, ZX and Peterson, VK, Direct Evidence of Concurrent Solid-Solution and Two-Phase Reactions and the Nonequilibrium Structural Evolution of $LiFePO_4$, J. Am. Chem. Soc. 134(18), 7867-7873 (2012) (from WOMBAT)

135. Shrestha, AK; Blazek, J; Flanagan, BM; Dhital, S; Larroque, O; Morell, MK; Gilbert, EP and Gidley, MJ, Molecular, mesoscopic and microscopic structure evolution during amylase digestion of maize starch granules, Carbohydr. Polym. 90(1), 23-33 (2012) (from Bruker (SAXS))

136. Shueh, C; Chen, PS; Cortie, D; Klose, F; Chen, WC; Wu, TH; van Lierop, J and Lin, KW, Correlating Uncompensated Antiferromagnetic Moments and Exchange Coupling Interactions in Interface Ion-Beam Bombarded $Co_{90}Fe_{10}$/CoFe-Oxide Bilayers, Jpn. J. Appl. Phys. 51(11), Art. No. PG102 (2012)

137. Shueh, C; Cortie, DL; Klose, F; van Lierop, J and Lin, KW, Modulating the Magneto-Crystalline Anisotropy and the Exchange Bias Field in CoFe/(Co,Fe)O Bilayers Using Ion-Beam Bombardment and Single Crystalline Substrates, IEEE T. Magn. 48(11), 2892-2895 (2012)

138. Simons, H; Glaum, J; Daniels, JE; Studer, AJ; Liess, A; Rodel, J and Hoffman, M, Domain fragmentation during cyclic fatigue in 94%$Bi_{(1/2)}Na_{(1/2)}$TiO3-6%$BaTiO_3$, J. Appl. Phys. 112(4), Art. No. 44101 (2012) (from WOMBAT)

139. Smith, ARG; Lee, KH; Nelson, A; James, M; Burn, PL and Gentle, IR, Diffusion - the Hidden Menace in Organic Optoelectronic Devices, Adv. Mater. 24(6), 822-826 (2012) (from NDF - Chemical Deuteration, PLATYPUS, X-ray reflectometer)

140. Spencer, K; Luzin, V; Matthews, N and Zhang, MX, Residual stresses in cold spray Al coatings: The effect of alloying and of process parameters, Surface and Coatings Technology 206(19-20), 4249-4255 (2012) (from KOWARI)

141. Stadler, AM; Garvey, CJ; Bocahut, A; Sacquin-Mora, S; Digel, I; Schneider, GJ; Natali, F; Artmann, GM and Zaccai, G, Thermal fluctuations of haemoglobin from different species: adaptation to temperature via conformational dynamics, J. R. Soc. Interface 9(76), 2845-2855 (2012)

142. Stapleton, A; Vaughan, B; Xue, BF; Sesa, E; Burke, K; Zhou, XJ; Bryant, G; Werzer, O; Nelson, A; Kilcoyne, ALD; Thomsen, L; Wanless, E; Belcher, W and Dastoor, P, A multilayered approach to polyfluorene water-based organic photovoltaics, Solar Energy Materials and Solar Cells 102, 114-124 (2012) (from X-ray reflectometer)

143. Stock, C; Broholm, C; Zhao, Y; Demmel, F; Kang, HJ; Rule, KC and Petrovic, C, Magnetic Field Splitting of the Spin Resonance in $CeCoIn_5$, Phys. Rev. Lett. 109(16), Art. No. 7207 (2012)

144. Sullivan, E; Avdeev, M and Vogt, T, Structural Distortions in $Sr_{3-x}A_xMO_4F$ (A=Ca, Ba; M=Al, Ga, In) Anti-Perovskites and Corresponding Changes in Photoluminescence, J. Solid State Chem. 194, 297-306 (2012) (from ECHIDNA)

145. Susilo, RA; Muñoz Pérez, S; Cobas, R; Cadogan, JM and Avdeev, M, Magnetic order and spin-reorientation in HoGa, J. Phys.: Conf. Ser. 340(1), Art. No. 012071 (2012) (from ECHIDNA)

146. Tan, TY; Kennedy, BJ; Zhou, QD; Ling, CD; Miiller, W; Howard, CJ; Carpenter, MA and Knight, KS, Impact of Jahn-Teller active Mn^{3+} on strain effects and phase transitions in $Sr_{0.65}P_{r0.35}MnO_3$, Physical Review B 85(10), Art. No. 104107 (2012)

147. Taylor, JE; Chow, JYH; Jeffries, CM; Kwan, AH; Duff, AP; Hamilton, WA and Trewhella, J, Calmodulin Binds a Highly Extended HIV-1 MA Protein That Refolds Upon Its Release, Biophys. J. 103(3), 541-549 (2012) (from NDF - Biodeuteration, QUOKKA)

148. Thomas, LH; Cheung, E; Jones, AOF; Kallay, AA; Lemée-Cailleau, M-H; McIntyre, GJ and Wilson, CC, 4-Phenoxyphenol: A Porous Molecular Material, Cryst. Growth Des 12(4), 1746-1751 (2012)

149. Tong, X; Jiang, CY; Lauter, V; Ambaye, H; Brown, D; Crow, L; Gentile, TR; Goyette, R; Lee, WT; Parizzi, A and Robertson, JL, In situ polarized ^{3}He system for the Magnetism Reflectometer at the Spallation Neutron Source, Rev. Sci. Instrum. 83(7), Art. No. 75101 (2012)

150. Toth, S; Lake, B; Hradil, K; Guidi, T; Rule, KC; Stone, MB and Islam, ATMN, Magnetic Soft Modes in the Distorted Triangular Antiferromagnet α-CaCr2O4, Phys. Rev. Lett. 109(12), Art. No. 127203 (2012)

151. Tremsin, AS; McPhate, JB; Steuwer, A; Kockelmann, W; M Paradowska, A; Kelleher, JF; Vallerga, JV; Siegmund, OHW and Feller, WB, High-Resolution Strain Mapping Through Time-of-Flight Neutron Transmission Diffraction with a Microchannel Plate Neutron Counting Detector, Strain 48(4), 296-305 (2012)

152. Turner, DR; Edwards, AJ and Piltz, RO, Nitrile groups as hydrogen-bond acceptors in a donor-rich hydrogen-bonding network, CrystEngComm 14(20), 6447-6451 (2012) (from Koala)

153. Turski, M; Paradowska, A; Zhang, S-Y; Mortensen, D; Fjaer, H; Grandfield, J; Davis, B and DeLorme, R, Validation of Predicted Residual Stresses within Direct Chill Cast Magnesium Alloy Slab, Metall. Mater. Trans. A 43(5), 1547-1557 (2012)

154. Veder, J-P; Patel, K; Sohail, M; Jiang, SP; James, M and de Marco, R, An Electrochemical Impedance Spectroscopy/ Neutron Reflectometry Study of Water Uptake in the Poly(3,4-Ethylenedioxythiop hene):Poly(Styrene Sulfonate)/Polymethyl Methacrylate-Polydecyl Methacrylate Copolymer Solid-Contact Ion-Selective Electrode, Electroanalysis 24(1), 140-145 (2012) (from PLATYPUS)

155. Waerenborgh, JC; Tsipis, EV; Pereira, LCJ; Avdeev, M; Naumovich, EN and Kharton, VV, Magnetization, Mossbauer and isothermal dilatometric behavior of oxidized $YBa(Co,Fe)_4O_{(7+delta)}$, Dalton Trans. 41(2), 667-678 (2012)

156. Wakeham, D; Niga, P; Ridings, C; Andersson, G; Nelson, A; Warr, GG; Baldelli, S; Rutland, MW and Atkin, R , Surface structure of a “non-amphiphilic” protic ionic liquid, Phys. Chem. Chem. Phys. 14(15), 5106-5114 (2012) (from Computing Cluster, X-ray reflectometer)

157. Walsh, RB; Howard, SC; Nelson, A; Skinner, WM; Liu, G and Craig, VSJ, Model Surfaces Produced by Atomic Layer Deposition, Chem. Lett. 41(10), 1247-1249 (2012) (from X-ray reflectometer)

158. Walsh, RB; Nelson, A; Skinner, WM; Parsons, D and Craig, VSJ, Direct Measurement of van der Waals and Diffuse Double-Layer Forces between Titanium Dioxide Surfaces Produced by Atomic Layer Deposition, J. Phys. Chem. C 116(14), 7838-7847 (2012) (from X-ray reflectometer)

159. Wang, CK; Wacklin, HP and Craik, DJ, Cyclotides Insert into Lipid Bilayers to Form Membrane Pores and Destabilize the Membrane through Hydrophobic and Phosphoethanolamine-specific Interactions, J. Biol. Chem. 287(52), 43884-43898 (2012) (from NDF - Biodeuteration)

160. Wang, JL; Campbell, SJ; Hofmann, M; Hoelzel, M; Zeng, R; Dou, SX and Kennedy, SJ, Structural properties and magnetic phase transition in $HoNi_2Mn$ ^{57}Fe, J. Appl. Phys. 111(7), Art. No. 07E334 (2012) (from WOMBAT)

161. Wang, JL; Campbell, SJ; Kennedy, SJ; Dou, SX and Wu, GH, $DyNi_2Mn$ - magnetisation and Mössbauer spectroscopy, Hyperfine Interactions 208(1-3), 43-48 (2012)

162. Wang, JL; Studer, AJ; Kennedy, SJ; Zeng, R; Dou, SX and Campbell, SJ, Magnetovolume effect in $Ho_2Fe_{(17-x)}Mn_x$ compounds, J. Appl. Phys. 111(7), Art. No. 07A911 (2012) (from WOMBAT)

163. Wang, S; Blazek, J; Gilbert, E and Copeland, L, New insights on the mechanism of acid degradation of pea starch, Carbohydr. Polym. 87(3), 1941-1949 (2012) (from Bruker (SAXS))

164. Wang, ZY; Garbe, U; Li, HJ; Studer, AJ; Harrison, RP; Callaghan, MD; Wang, YB and Liao, XZ, Hydrogen-induced microstructure, texture and mechanical property evolutions in a high-pressure torsion processed zirconium alloy, Scr. Mater. 67(9), 752-755 (2012) (from WOMBAT)

165. Webster, NAS; Loan, MJ; Madsen, IC; Knott, RB; Brodie, GM and Kimpton, JA, An in situ synchrotron X-ray diffraction investigation of lepidocrocite and ferrihydrite-seeded $Al(OH)_3$ crystallisation from supersaturated sodium aluminate liquor, J. Cryst. Growth 340(1), 112-117 (2012)

166. Wensrich, CM; Kisi, EH; Zhang, JF and Kirstein, O, Measurement and analysis of the stress distribution during die compaction using neutron diffraction, Granular Matter (2012)

167. Whitfield, R; Goossens, D; Studer, A and Forrester, J, Measuring Single-Crystal Diffuse Neutron Scattering on the WOMBAT High-Intensity Powder Diffractometer, Metall. Mater. Trans. A 43(5), 1423-1428 (2012) (from WOMBAT)

168. Wildes, AR; Rule, KC; Bewley, RI; Enderle, M and Hicks, TJ, The magnon dynamics and spin exchange parameters of $FePS_3$, Journal Of Physics-Condensed Matter 24(41), Art. No. 16004 (2012)

169. Willenberg, B; Schäpers, M; Rule, KC; Süllow, S; Reehuis, M; Ryll, H; Klemke, B; Kiefer, K; Schottenhamel, W; Büchner, B; Ouladdiaf, B; Uhlarz, M; Beyer, R; Wosnitza, J and Wolter, AUB, Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite $PbCuSO_4(OH)_2$, Phys. Rev. Lett. 108(11), Art. No. 117202 (2012)

170. Witt, T; Doutch, J; Gilbert, EP and Gilbert, RG, Relations between Molecular, Crystalline, and Lamellar Structures of Amylopectin, Biomacromolecules 13(12), 4273-4282 (2012) (from Bruker (SAXS))

171. Wolter, AUB; Lipps, F; Schäpers, M; Drechsler, SL; Nishimoto, S; Vogel, R; Kataev, V; Büchner, B; Rosner, H; Schmitt, M; Uhlarz, M; Skourski, Y; Wosnitza, J; Süllow, S and Rule, KC, Magnetic properties and exchange integrals of the frustrated chain cuprate linarite $PbCuSO_4(OH)_2$, Physical Review B 85(1), Art. No. 014407 (2012)

172. Xia, F; Brugger, J; Qian, G; Ngothai, Y; O'Neill, B; Zhao, J; Pullen, S; Olsen, S and Pring, A, Single-pass flow-through reaction cell for high-temperature and high-pressure in situ neutron diffraction studies of hydrothermal crystallization processes, J. Appl. Crystallogr. 45(2), 166-173 (2012) (from WOMBAT)

173. Yahia, HB; Shikano, M; Koike, S; Tatsumi, K; Kobayashi, H; Kawaji, H; Avdeev, M; Miiller, W; Ling, CD; Liu, J and Whangbo, M-H, Synthesis and Characterization of the Crystal Structure and Magnetic Properties of the New Fluorophosphate $LiNaCo[PO_4]F$, Inorg. Chem. 51(16), 8729-8738 (2012) (from ECHIDNA)

174. Yahia, HB; Shikano, M; Sakaebe, H; Koike, S; Tabuchi, M; Kobayashi, H; Kawaji, H; Avdeev, M; Miiller, W and Ling, CD, Synthesis and characterization of the crystal structure, the magnetic and the electrochemical properties of the new fluorophosphate $LiNaFe[PO_4]F$, Dalton Trans. 41(38), 11692-11699 (2012) (from ECHIDNA)

175. Yajima, T; Nakano, K; Takeiri, F; Ono, T; Hosokoshi, Y; Matsushita, Y; Hester, J; Kobayashi, Y and Kageyama, H, Superconductivity in $BaTi_2Sb_2O$ with a d1 Square Lattice, J. Phys. Soc. Jpn. 81(10), Art. No. 3706 (2012) (from ECHIDNA)

176. Yang, P-W; Lin, T-L; Liu, IT; Hu, Y and James, M, In situ neutron reflectivity studies of the adsorption of DNA by charged diblock copolymer monolayers at the air-water interface, Soft Matter 8(27), 7161-7168 (2012) (from PLATYPUS)

177. Yang, XS; Yuan, LX; Peterson, VK; Minett, AI; Yin, YB and Harris, AT, Facile Preparation of Free-Standing Carbon Nanotube Arrays Produced Using Two-Step Floating-Ferrocene Chemical Vapor Deposition, ACS Appl. Mater. Interfaces 4(3), 1417-1422 (2012)

178. Yao, SH; Sang, YH; Yu, DH; Avdeev, M; Liu, H; Wang, JY and Zhang, NN, Low Temperature Neutron Diffraction on Congruent and Near Stoichiometric $LiNbO_3$, Mod. Phys. Lett. B 26(22), Art. No. 50142 (2012) (from ECHIDNA)

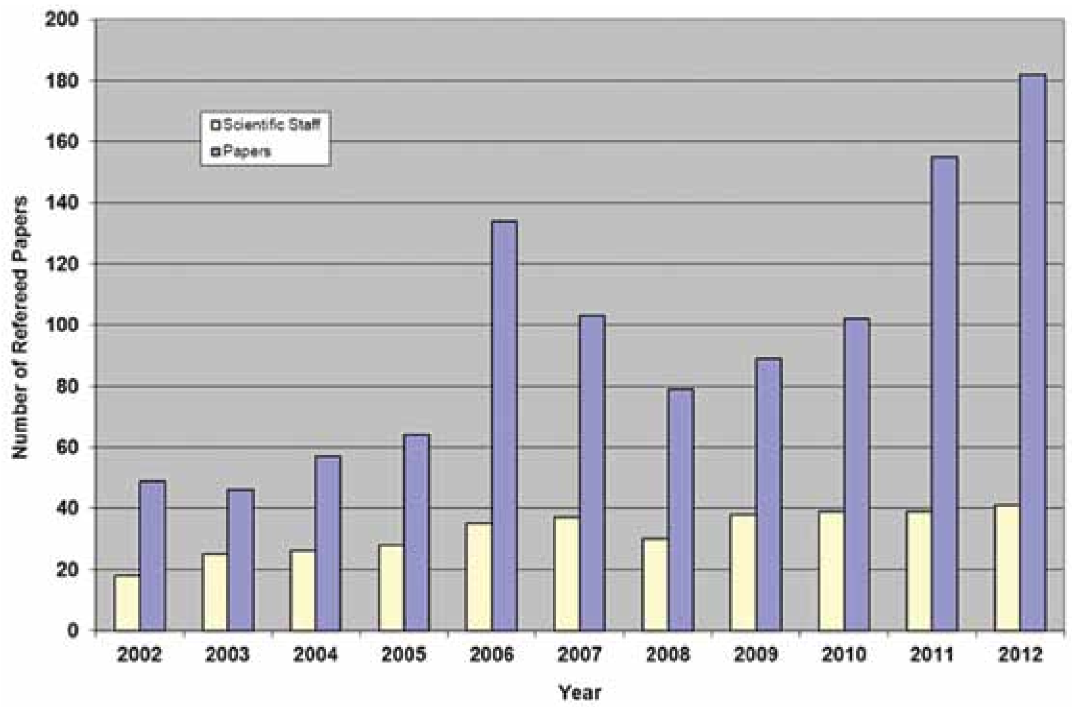
179. Yibmantasiri, P; Leahy, DC; Busby, BP; Angermayr, SA; Sorgo, AG; Boeger, K; Heathcott, R; Barber, JM; Moraes, G; Matthews, JH; Northcote, PT; Atkinson, PH and Bellows, DS, Molecular basis for fungicidal action of neothyonidioside, a triterpene glycoside from the sea cucumber, Australostichopus mollis, Molecular BioSystems 8(3), 902-912 (2012)

180. Zhao, M; Yang, X; Church, TL and Harris, AT, Novel CaO-SiO_2 Sorbent and Bifunctional Ni/Co-CaO/SiO_2 Complex for Selective H2 Synthesis from Cellulose, Environmental Science & Technology 46(5), 2976-2983 (2012)

181. Zhou, QD; Blanchard, P; Kennedy, BJ; Reynolds, E; Zhang, ZM; Miiller, W; Aitken, JB; Avdeev, M; Jang, LY and Kimpton, JA, Synthesis, Structural and Magnetic Studies of the Double Perovskites Ba_2CeMO_6 (M = Ta, Nb), Chem. Mater. 24(15), 2978-2986 (2012) (from ECHIDNA)

182. Zhu, PN; Wu, YZ; Reddy, MV; Nair, AS; Peng, S; Sharma, N; Peterson, VK; Chowdari, BVR and Ramakrishna, S, TiO_2 nanoparticles synthesized by the molten salt method as a dual functional material for dye-sensitized solar cells, RSC Advances 2(12), 5123-5126 (2012) (from WOMBAT)

Indicators for Bragg Institute 2002-2012



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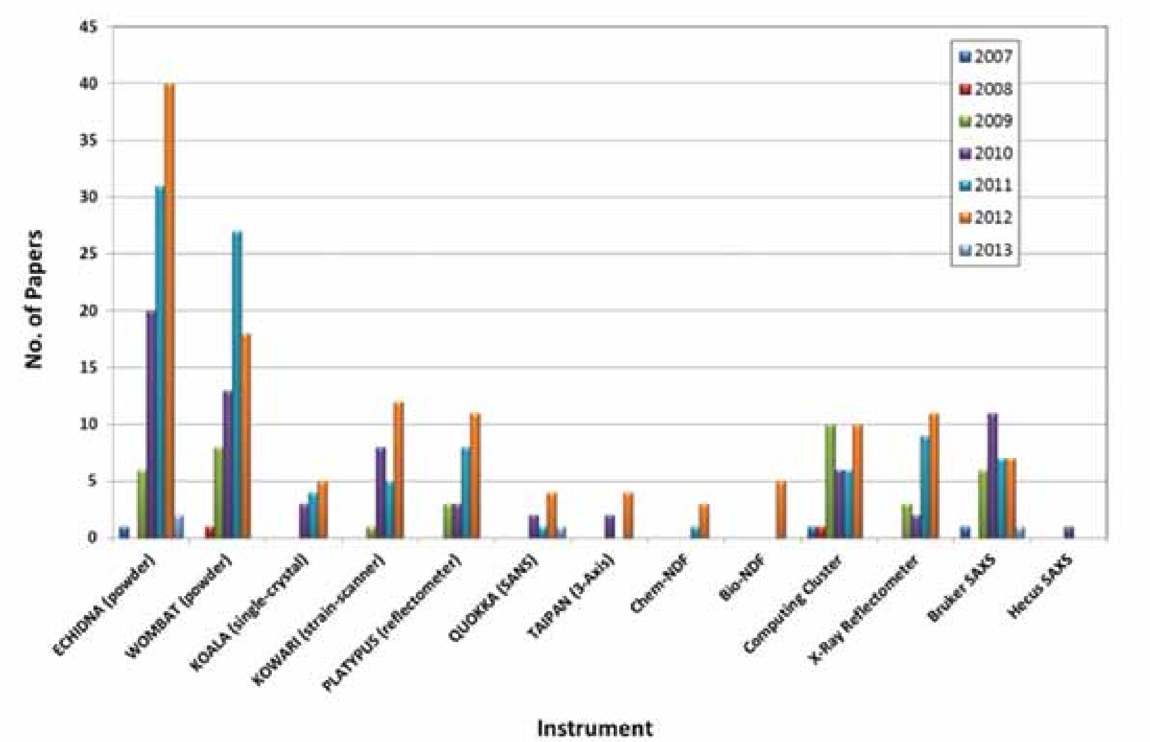
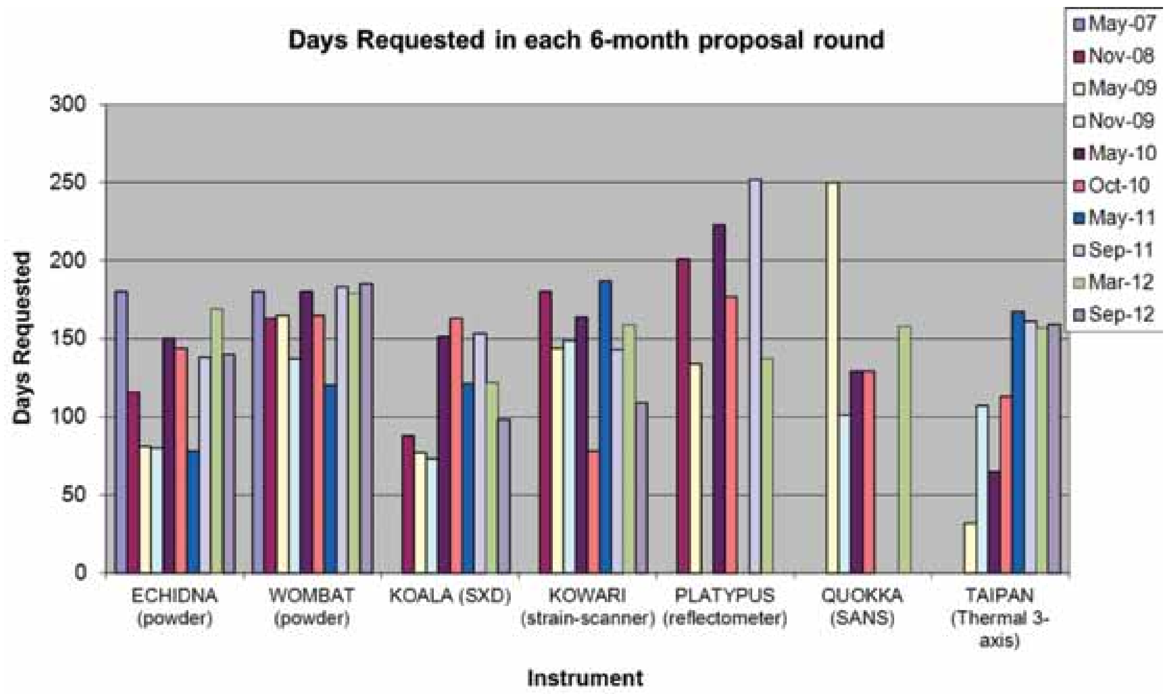
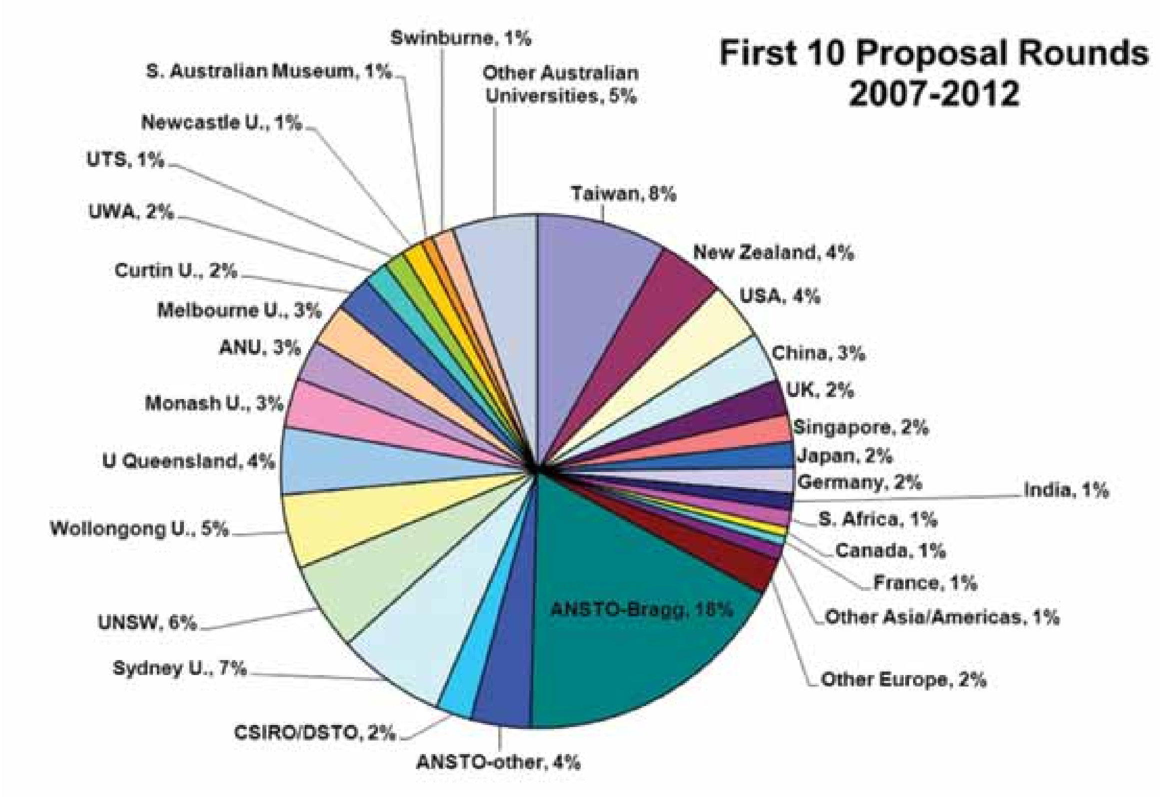


Papers produced from the user programs at OPAL and the National Deuteration Facility, computing cluster and the Institute's three in-house X-ray instruments.

Subscription Rates and Inverse Success Rates for the User Program at OPAL from Rounds 2 -12 (November 2008 – September 2012). Subscription Rate = number of days requested (including pre-existing programs and an estimate of mail-in business on ECHIDNA) divided by number of days available (typically 200 days per year); Success Rate = number of days recommended for approval by Program Advisory Committee, divided by number requested in proposals. The main difference is that there has been some carry-over between rounds, due to reactor, cold-source and other equipment problems, and that on occasion, the Program Advisory Committee has not awarded all available beam time, as insufficient proposals have met the minimum quality or feasibility standard.



Demands (in days) by instruments, over all 10 proposal rounds to date. Each round covers a 6-month period, and a maximum of 100 days per instrument is typically awarded.



Geographical breakdown of demand for neutrons at OPAL over all rounds to date.

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