

# **AINSE**

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## ***AINSE's 50<sup>th</sup> Anniversary Seminar***

***1958 - 2008***

Friday 12 December 2008  
Lucas Heights, Sydney

***Celebrating 50 years of relevance***

## Foreword

This seminar contributes to the celebration of the 50<sup>th</sup> anniversary of AINSE on 4 December 2008.

One of the strengths of AINSE in the last 50 years has been its encouragement and support of young researchers in nuclear science and engineering and in related fields. Many of these scientists have since gone on to make their mark in the Australian and international scientific communities.

In this seminar, we continue this encouragement by featuring the most recent cohort of AINSE research students and fellows, giving a snapshot of current research being supported by AINSE. The presentations in this seminar cover bioscience, materials science and environmental science. They involve techniques including neutron scattering, accelerators, and natural radioactivity. The research embodies both novelty and relevance.

The seminar is opened by ANSTO Chairman Dr Ziggy Switkowski, himself a recipient of AINSE support, when, as a research student under Dr Graham Sargood in the School of Physics at the University of Melbourne, he conducted experiments on the 3 MeV Van de Graaff accelerator to study  $^{23}\text{Na}(p,g)^{24}\text{Mg}$  and other reactions of astrophysical significance.

AINSE has evolved over fifty years and expects to continue to grow and develop, meeting the challenges of supporting scientific research in a changing world.

# AINSE 50<sup>th</sup> Anniversary

## Seminar Timetable

0930 – 0945	<b>Welcome: Professor Allan Chivas, President, AINSE</b>	
0945 – 1000	<b>Opening Remarks: Dr Ziggy Switkowski, Chairman, ANSTO</b>	
1000 – 1015	<b>Dr Duncan McGillivray, University of Auckland, AINSE Research Fellow</b> Proteins at the edge: biological membrane – protein interactions through neutron reflectometry	1
1015 – 1030	<b>Mr Mark Callaghan, University of Wollongong, ex AINSE PGRA</b> A study of the high temperature fatigue behaviour and life prediction of 2.25Cr-1Mo Alloy Steel	2
1030 – 1045	<b>Ms Tara Busbridge, Griffith University, AINSE PGRA</b> <i>In situ</i> x-ray investigation of CO <sub>2</sub> densification in coal	3
1045 – 1115	Morning Tea	
1115 – 1130	<b>Dr Moeava Tehei, University of Wollongong, AINSE Research Fellow</b> Neutron scattering reveals adaptation to extreme environments	4
1130 – 1145	<b>Mr David A Jacques, The University of Sydney, ex AINSE PGRA</b> Probing bacterial signalling with small-angle scattering	5
1145 – 1200	<b>Mr Alan Burt, Griffith University, AINSE PGRA</b> <i>In situ</i> neutron powder diffraction study of hydrogen storage in the LiBH <sub>4</sub> +MgH <sub>2</sub> system	6
1200 – 1215	<b>Mr Ben Kent, RMIT, AINSE PGRA</b> Towards a molecular mechanism for the protective effects of sugars on membrane damage during dehydration	7
1215 – 1230	<b>Mr Ryan Mills, University of Melbourne, AINSE PGRA</b> Domain organisation in solution of the monomeric form of the Tom70 mitochondrial import receptor	8
1230 – 1245	<b>Dr Darren Goossens, Australian National University, AINSE Research Fellow</b> Recent progress in the Structure and Magnetism of Materials Group at ANU	9
1245 – 1345	Lunch	
1345 – 1400	<b>Dr Helen McGregor, University of Wollongong, AINSE Research Fellow</b> El Niño in context: reading the coral record of past climate extremes	10
1400 – 1415	<b>Ms Amy Wyatt, University of Wollongong, AINSE PGRA</b> The role of clusterin in extracellular protein folding quality control	11
1415 – 1430	<b>Dr Matthias Raiber, GNS, ex AINSE PGRA</b> Using age dating to study groundwater dynamics in the basalt plains of western Victoria	12
1430 – 1445	<b>Dr Katherine Lilly, University of Otago, ex AINSE PGRA</b> Pleistocene changes in East Antarctic ice sheet thickness as observed with cosmogenic nuclide measurements	13

1445 – 1500	<b>Ms Amy Ziebell, University of Wollongong, AINSE PGRA</b> Characterisation of a 2 <sup>nd</sup> generation silicon-on-insulator microdosimeter	14
1500 – 1530	Afternoon Tea	
1530 – 1545	<b>Dr Daniel Riley, University of Melbourne, AINSE research fellow</b> Application of crystalline precursors to the design of novel materials	15
1545 – 1600	<b>Ms Betime Nuhiji, Deakin University, AINSE PGRA</b> Structure property relationships in thermosetting epoxy nanocomposites	16
1600 – 1615	<b>Dr Catherine Kealley, UTS, ex AINSE PGRA</b> Determination of the structure of a gold-based shape memory alloy	17
1615 – 1630	<b>Dr Lizhong He, University of Queensland, AINSE Research Fellow</b> Neutron reflection study of stimuli-response peptides at the air-water interface	18
1630 – 1645	<b>Closing Comments: Professor Bruce King, Vice President, AINSE</b>	



# Proteins at the edge: biological membrane – protein interactions through neutron reflectometry

Duncan McGillivray

*Lecturer / AINSE Research Fellow*

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Cellular membranes, and their interactions with intra- and extra-cellular constituents such as proteins and peptides, are crucial features in many biological problems. However, they are complex systems that are not readily probed using conventional techniques. Using a biomimetic solid-supported membrane system, many of the features of natural membranes can be created in a controlled fashion in a system which is amenable to quantitative analysis, particularly using the strengths of neutron reflectometry.

I shall describe a flexible and robust membrane system we have developed and characterised for membrane-protein studies. Using this system we have studied membrane pore-forming proteins (e.g.,  $\alpha$ -haemolysin) and the Alzheimer's related  $\beta$ -amyloid peptides, giving information about their membrane incorporated structures, and will continue to study the mode of activity of anti-microbial proteins as new opportunities for drug development

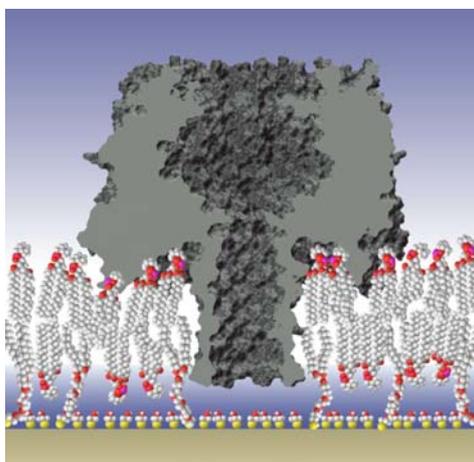


Figure 1: A cartoon of an  $\alpha$ -haemolysin pore incorporated in a biomimetic membrane

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# **A study of the high-temperature fatigue behaviour and life prediction of 2.25Cr-1Mo alloy steel**

Mark D Callaghan  
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In the 21<sup>st</sup> Century, power generation requirements are heavily influenced by daily energy demands. To satisfy variable energy requirements, power plants that were designed originally to operate under a steady-state base load are now subjected to loading cycles. Loading cycles expose components to both mechanical and thermal stresses and strains not encountered during steady-state operation which may have a detrimental effect on mechanical properties including fatigue resistance and endurance life.

The aim of this research was to characterise and compare the high-temperature fatigue behaviour of 2.25Cr-1Mo alloy steel, used in the nuclear and fossil-fuelled power generation industry, using two fatigue specimens (standard-sized and miniature) of different geometries. This research involved two aspects: The design, development and validation of a high-temperature fatigue testing system and methodology to produce accurate fatigue data; and the characterisation and modelling of the high-temperature fatigue properties through strain-based and energy-based approaches, by use of the data obtained. Analytical methods were also undertaken to provide fatigue data for these approaches and to further evaluate the fatigue properties. The results showed that the fatigue behaviour of the test material characterised by the miniature specimen, compared well with that of the standard-sized specimen and previous literature.

## ***In situ* x-ray investigation of CO<sub>2</sub> densification in coal**

Tara Busbridge  
*Griffith University*

Carbon sequestration in unmineable coal seams is a proposed interim measure for slowing the rising concentration of atmospheric carbon dioxide. To estimate reservoir capacities, injection rates and storage stability, a better understanding of coal-CO<sub>2</sub> interactions and the mechanism of sorption is required. Here, the results of a small angle x-ray scattering experiment on a sample taken from a potential sequestration site, the Baralaba coal seam, Bowen Basin, QLD, are presented. The time- and position-resolved data give insight into the CO<sub>2</sub> sorption in the micro- and small mesopores. The results indicate that the CO<sub>2</sub> preferentially invaded the smallest micropores and the confined CO<sub>2</sub> density was up to five times that of the free CO<sub>2</sub>. Faster sorption kinetics was found in regions containing a greater abundance of mineral matter but, the mineral-matter-rich regions had lower-density CO<sub>2</sub> in their pores. The technique presented here not only offers the potential to enhance the understanding of the storage of CO<sub>2</sub> in coal but can also be broadly applied to investigate the interaction of invading fluids with porous media of any kind.

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## Neutron scattering reveals adaptation to extreme environments

Moeava Tehei

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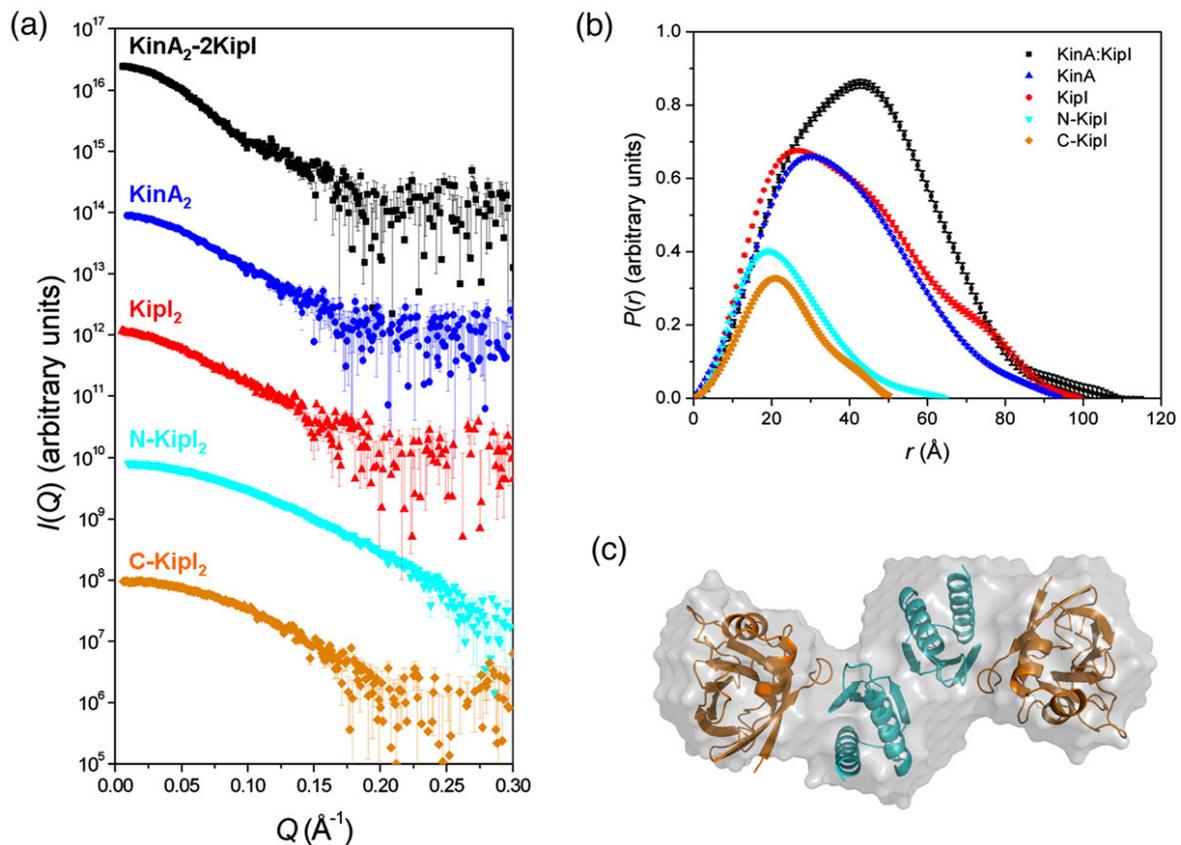
Organisms can thrive in what we call extreme environments on Earth and perhaps elsewhere in the Solar System. Macelroy named these lovers ('philos' to Greeks) of extreme environments 'extremophiles'. They had to adapt to one or several physico-chemical extreme parameters: high temperatures for thermophiles that live above 60°C near geysers and hydrothermal vents, whereas psychrophiles grow at temperatures below 15°C in glacier water and polar seas. Halophiles thrive in hypersaline environments such as the Lac Rose in Senegal. Other examples of physico-chemical extreme parameters are high pressure, high radiation activity, high and low pH. Research on extremophiles has intensified in recent years due to both their practical and fundamental significance. On the practical side, the extremophiles and their enzymes have an important economic potential in multiple areas (detergent manufacturing, bioscavengers, ...), either by direct applications for catalysis under extreme conditions or by tapping them as sources of ideas to modify mesophile enzymes (adapted to 'normal' physico-chemical conditions), with the aim of improving their properties and stability at high temperature, for example. On the fundamental side, a comparison of thermophilic proteins with their mesophile counterparts, for example, can help to increase our understanding of the physico-chemical basis of protein stability. The study of extremophile adaptation has also broad implications for exobiology. Using neutron scattering experiments, we have measured molecular dynamics for thermophilic enzyme, immobilized enzyme resistant to extreme temperatures and dynamics of water inside halophile cells adapted to hyper-saline conditions. We have demonstrated that molecular dynamics presents one of these molecular mechanisms of adaptation.

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# Probing bacterial signalling with small-angle scattering

David A Jacques  
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The sensor histidine kinase A (KinA) from *Bacillus subtilis* triggers a phosphorelay that activates sporulation. The antikinase Kipl prevents sporulation by binding KinA and inhibiting the autophosphorylation reaction. Using neutron contrast variation, mutagenesis, and fluorescence data, we have shown that two Kipl monomers bind via their C-domains at a conserved proline in the KinA dimerization and histidine-phosphotransfer (DHP) domain. Our crystal structure of the Kipl C-domain reveals the binding motif has a distinctive hydrophobic groove formed by a five-stranded antiparallel  $\beta$ -sheet; a characteristic of the cyclophilin family of proteins that bind prolines and often act as cis-trans peptidyl-prolyl isomerases. We have proposed that the DHP domain of KinA transmits conformational signals to regulate kinase activity via this proline-mediated interaction. Given that both KinA and Kipl homologues are widespread in the bacterial kingdom, this mechanism has broad significance in bacterial signal transduction. The significance of this discovery is highlighted by the fact that cyclophilin-like inhibitors have never previously been implicated in the regulation of histidine kinase signalling systems.



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## ***In situ* neutron powder diffraction study of hydrogen storage in the $\text{LiBH}_4 + \text{MgH}_2$ system**

Edmund Alan Burt, Matthew Crossley, Jim Webb, Evan Gray  
*Nanoscale Science and Technology Centre Griffith University*

Hydrogen is a light, clean energy vector however the means of storing hydrogen with sufficient energy density has yet to be found after many years of intense research. The 2:1 mixture of  $\text{LiBH}_4$  and  $\text{MgH}_2$  is seen as a promising condensed matter hydrogen storage system, releasing wt% H at temperatures above  $275^\circ\text{C}$ , the melting point of  $\text{LiBH}_4$ . Here, we present the results of two in-situ neutron diffraction experiments on the hydrogenation of 2:1 mixtures of LiH and  $\text{MgB}_2$  using  $\text{VCl}_3$  and titanium isopropoxide additives. Diffraction was performed on the POLARIS instrument at ISIS with hydrogenation conditions of  $250^\circ\text{C}$  and 500 bar hydrogen gas pressure. Results show the slow conversion upon hydrogen uptake of  $\text{LiH} + \text{MgB}_2$  into  $\text{LiBH}_4 + \text{MgH}_2$ . This is the lowest temperature at which this reaction has been observed to proceed.

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# Towards a molecular mechanism for the protective effects of sugars on membrane damage during dehydration

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In healthy biological tissue, most membranes exist in a fluid bilayer phase. The fluid bilayer structure is critical for maintaining cell structure and function. However, when biological cells are dehydrated or slowly frozen, the cells contract osmotically, and the membranes (both bounding and internal) are brought into close proximity. This close approach leads to a compressive stress in the membranes which can induce membrane phase transitions into other lipid phases which are not favourable for normal biological function. Such phases include the gel phase (where lipid chains are frozen) and various inverse phases, such as the inverse hexagonal phase. Transitions to such phases are always deleterious to biological function, and are often lethal for cells.

Some organisms have evolved the ability to increase their tolerance to dehydration and freezing by accumulating small solutes (eg sugars) which stabilise membranes against deleterious phase transitions. The phase behaviour and transition kinetics of membranes in the presence of sugars is therefore of primary importance in understanding freezing and dehydration damage.

This talk will present results from small angle x-ray scattering (SAXS) and small angle neutron scattering (SANS) experiments which aim to determine how sugars affect transitions to non-bilayer inverse phases, such as the inverse hexagonal phase. These results will be discussed in terms of our current understanding of how sugars protect membranes during dehydration.

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## Domain organization in solution of the monomeric form of the Tom70 mitochondrial import receptor

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The TOM (translocase of the outer membrane) complex is responsible for the transport of proteins across the mitochondrial outer membrane. The large receptor subunit Tom70 is composed of N- and C-terminal domains that bind chaperones and mitochondrial precursors, respectively. In yeast, the C-terminal tails of cytosolic Hsp70 family chaperones bind to the N-terminal 'clamp' domain of Tom70 delivering chaperone-bound precursors to the TOM complex for import. To better understand how Tom70 interacts with chaperones and precursors we have studied the solution structure of yeast Tom70 using small-angle x-ray scattering (SAXS). The SAXS data indicate that the isolated cytosolic region of Tom70 exists in solution as an elongated monomer. Poor fits were obtained when the SAXS data were compared with the theoretical scattering profiles from the dimer or 'closed' monomers identified in the Tom70 crystal structure (Wu and Sha (2006) *Nat Struct Mol Biol.* 13(7):589-93). Monomer in an alternate 'open' domain arrangement fits the experimental SAXS data considerably better. Upon addition of a peptide corresponding to the C-terminal tails of the yeast cytosolic Hsp70s, the fit of the SAXS data to the open monomer improves further. We also report that the open monomer can bind precursor peptides derived from the yeast mitochondrial inner membrane phosphate carrier protein Mir1/PiC, that precursor-binding is independent of Hsp70 tail-binding, and Hsp70-binding is incompatible with dimerization. Our data suggest a model for the delivery of chaperone-bound precursors to the TOM complex, where both chaperone and precursor are received by open Tom70 monomers.

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## Recent progress in the Structure and Magnetism of Materials Group at ANU

Darren Goossens

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This presentation will outline some of the research that has taken place in the recently established Structure and Magnetism of Materials Group in the Research School of Chemistry at ANU. The group was begun in 2007 when the AINSE fellowship began, but has really taken shape in 2008 with the work of two honours students and two undergraduate project students.

Jessica Hudspeth's Honours degree centred on the structural and magnetic properties of rare-earth calcium ferrates. This project was done in collaboration with the Bragg Institute, UNSW@ADFA and several units within the ANU. Jessica established the crystal structure and magnetic ordering in an important family of perovskite-related structures by using a combination of X-ray, electron and neutron diffraction, as well as other techniques like Mössbauer spectroscopy.

Ross Whitfield's Honours project used *in situ* neutron diffraction on Wombat at the Bragg Institute to look at the sintering of metal injection moulded parts in real time, gaining new understanding of the dynamics of crystal phase formation during the sintering process. Ross intends to work with the group next year as a Ph.D. student, working on the short-range order in piezoelectric materials, a project for which we have obtained ARC funding.

Other work in the group includes studies of short-range order in molecular crystals and in functional oxides, and these will be briefly illustrated.

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## **El Niño in context: reading the coral record of past climate extremes**

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El Niño-Southern Oscillation (ENSO) is now recognised as the single most important source of global interannual climate variability. It is increasingly clear that ENSO is correlated with climate in the Australasian region, influencing flood and drought conditions. However our current knowledge of this crucial climate component is limited by the brevity of historical datasets, which span only the past 150 years. The modern records of ENSO must be supplemented with proxy data of past climate to quantify which trends in today's climate are part of a natural pattern, and to identify potential analogues of future climate. In this study geochemical ratios measured in corals are used to reconstruct past variations in frequency and magnitude of ENSO. The corals were collected from Kiritimati (Christmas) Island, Kiribati, which lies within the dry equatorial zone of the central Pacific. This island is particularly dry and desolate (average annual precipitation 936 mm), but lies on a steep precipitation and ocean surface temperature gradient, and receives heavy rainfall (eg 3686 mm during the 1997 El Niño) and marked changes in ocean temperature during El Niño events. This makes it uniquely sensitive to El Niño. Stable oxygen isotope ratios ( $\delta^{18}\text{O}$ ) measured in corals are an indirect yet quantifiable measure of changes in ocean temperature and salinity, parameters that define ENSO events.  $\delta^{18}\text{O}$  analyses of fossil corals from Christmas Island indicate that El Niño was less intense than present ~3000 years ago. In addition, the corals provide detailed evidence of multiple El Niño events occurring around 2000 years ago that were as extreme as the 1997 'event of the century'. The magnitude of these extreme El Niños is surprising since they occurred under different background ocean temperatures in the equatorial Pacific compared to present-day El Niños. The results confirm preliminary data from other locations and modelling evidence for more intense ENSO around 2000 years ago, allow us to unravel the underlying processes and mechanisms driving ENSO, and provide a much-needed ENSO baseline to investigate the likely ENSO behaviour under future greenhouse warming.

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## The role of clusterin in extracellular protein folding quality control

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Processes to attain and maintain the correct three-dimensional shape, or 'native conformation' of proteins are vital. However, certain conditions including thermal and oxidative stress may cause proteins to unfold and aggregate. Intracellular and/or extracellular protein aggregates have been identified in a large number of diseases, including Alzheimer's disease, arthritis and type II diabetes. While several intracellular quality control mechanisms for the folding state of proteins have been characterized, corresponding mechanisms that function extracellularly have yet to be identified. Clusterin is an extracellular chaperone that can stabilize proteins and prevent their precipitation during exposure to elevated temperatures or oxidative stress. We have demonstrated that clusterin stabilizes proteins by forming soluble high molecular weight (HMW) complexes ( $> 4 \times 10^7$  Da) with them. Using an animal model, the fate of blood-borne <sup>123</sup>I-HMW clusterin-stressed protein complexes was investigated. <sup>123</sup>I-HMW clusterin-stressed protein complexes were rapidly cleared from circulation and retained primarily in the liver and spleen compared to free clusterin and heated but uncomplexed control proteins. *In vitro* studies have shown that isolated hepatocytes bind HMW complexes and this binding is inhibited by fucoidin, a pan-specific ligand of scavenger receptors. In the absence of specific extracellular proteolytic mechanisms it appears likely that stress damaged extracellular proteins are targeted by clusterin and transported intracellularly by scavenger receptors for degradation. The findings of this study suggest an important role for clusterin in global extracellular protein quality control.

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## **Using age dating to study groundwater dynamics in the basalt plains of western Victoria**

Matthias Raiber  
*GNS Science*

Groundwater dating combined with other environmental tracers and geological information was used to investigate the geological controls on the spatial distribution of groundwater quality in a regional-scale basalt aquifer and an underlying palaeoriver system in the basalt plains of western Victoria. The present study shows that groundwaters recharged through major volcanoes are generally young, whereas groundwater ages away from this eruption points have maximum ages of more than 37000 years BP. The old groundwater ages clearly emphasise that these resources are essentially non-renewable on human time-scales, and that a sustainable management is required to preserve these groundwaters for future generations.

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# Pleistocene changes in East Antarctic ice sheet thickness as observed with cosmogenic nuclide measurements

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Current glaciology-based models which attempt to describe the spatial and temporal evolution of the East Antarctic Ice Sheet (EAIS) are poorly constrained by observations. Few data are available that can directly document past ice-volume variations, particularly for the interior sectors of the EAIS. Surface exposure dating using in situ-produced cosmogenic nuclides provides an ideal tool for identifying and dating former ice sheet margins and ice sheet thickness changes, including at sites where no other direct dating method is possible.

Cosmogenic radionuclide <sup>10</sup>Be and <sup>26</sup>Al concentrations measured in bedrock surfaces and glacially-transported material collected from the Grove Mountains provide new and direct age constraints on former ice sheet extent over the past three million years. The Grove Mountains are located at a high-altitude, inland site far from the coast and from fast-flowing ice streams.

Very high cosmogenic nuclide concentrations in both erratics and bedrock surfaces at Grove Mountains indicate that surface erosion rates have been extremely low over the Quaternary, with minimum exposure ages as high as 3 Ma measured. Interpretation of these exposure ages suggests that the ice surface elevation in interior East Antarctica has remained remarkably stable over the Quaternary. Measured bedrock exposure ages are successfully modelled only via a model which contains both a long-term thinning trend and shorter period oscillations. Moreover, there is no evidence that ice sheet thickness at Grove Mountains was greater at the Last Glacial Maximum than it is today.

Field observation and quantitative data are necessary to validate and test existing models of ice sheet history. Amongst the most poorly constrained aspects of EAIS history is former ice thickness, and the results presented here provide new and direct constraints on this during the Pleistocene.

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## Characterisation of a 2nd generation silicon-on-insulator microdosimeter

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**Introduction:** The microdosimetry approach infers the radiobiological properties of a mixed radiation field by measuring the energy deposited by the beam in a micron sized volume. Traditionally gas proportional counters have been used. These detectors have the advantage of excellent tissue equivalency of the gas but suffer from some well documented short comings. Silicon microdosimeters address several of these problems. Recently a silicon detector with a planar SV has been developed at the University of Wollongong's Centre for Medical Radiation Physics (CMRP). Studies have identified that the performance of the device may be improved upon by modifying the geometry of the SV from planar to cylindrical. Through the CMRP's collaboration with the University of New South Wales (UNSW) and the Australian Nuclear Science and Technology Organisation (ANSTO) such a cylindrical device has been fabricated and is currently being tested.

**Methods:** The charge collection characteristics of the new cylindrical silicon detector structure were experimentally determined via an ion beam induced charge (IBIC) study. This was performed using the heavy ion microprobe at ANSTO. The amount of energy deposited within the microdosimeter for each ion traversal,  $\Delta E$ , was measured with a standard charge sensitive preamplifier, shaping amplifier and MCA in coincidence with digitized voltage signals of the beam position,  $x$  and  $y$  for each event in  $\Delta E$ . Data triplets  $(x,y,\Delta E)$  were saved for each event in a list mode file. Analysis software was used to generate IBIC imaging maps displaying a spatially resolved image of the median amount of charge collected as a function of beam position.

**Results:** Results reveal that the new detector structures possess a well defined cylindrical SV. An array of these structures successfully provides a greater effective surface area without any degradation of the measured spectrum.

**Discussion and Conclusion:** Given that the second generation detector structures possess a well defined cylindrical SV, they have the potential to improve upon the performance of the previous silicon microdosimeter design.

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# Application of crystalline precursors to the design of novel materials

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Crystallographic sub-units common to binary and ternary compounds are the key to the optimised synthesis of complex laminate materials. Advances in the application of binary carbides as model systems for the synthesis of ternary MAX Phases has proven successful in significantly reducing processing times and temperatures, where  $M$  is an early transition metal,  $A$  is either a Group III or IV element and  $X$  is either C or N. This research has been recently complemented with *ab initio* DFT studies of the reaction, identifying the localised ordering of interstitial vacancies as the mechanism by which long-range intercalation of  $A$ -Group elements may occur. These findings have been correlated with the ordering of customised precursors,  $M_nX_{n+1} = TiC_{1-x}$ , during reaction with either Si or Al to form  $Ti_3SiC_2$  and  $Ti_3AlC_2$ , respectively. These results were obtained using time-resolved *in-situ* neutron diffraction, a technique also successfully applied to the study of self-propagating high-temperature synthesis (SHS) of MAX Phase materials. Comparisons between the intermediate phase formed during SHS,  $3TiC_{2/3}(1/3Si)$ , and the ordered precursor have confirmed that the reaction sequences are related, but nonetheless unique.

Overall, the application of time-resolved neutron diffraction has reduced the development time of this novel synthesis method, clearly illustrating the link between interstitial ordering and the increased inter-diffusion of the  $A$ -group elements. Previous studies have shown that the self-ordering of substoichiometric carbides takes an appreciable amount of time (1 month) at elevated temperatures ( $>1500^\circ C$ ). It is therefore proposed that the significantly quicker precursor route is initiated by surface intercalation of an  $A$ -Group atom, followed by strain pinning of additional carbon vacancies. Longer-range diffusion is therefore facilitated by the ordering of carbon vacancies, lowering the localised activation energy and enabling the synthesis of the lamella MAX Phase. On-going work has verified the wider applicability of this synthesis technique.

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# Structure property relationships in thermosetting epoxy nanocomposites

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The manufacture of inexpensive light weight materials for the aerospace and automotive industries is becoming more and more important as global issues such as high fuel prices and climate change affect the transport industry.

Since Toyota's pioneering work on Nylon 6/clay nanocomposites in the early 1990s <sup>[1]</sup>, a great deal of research has focussed on compounds of thermoplastic polymers and nanoparticles. This work steered the commercialisation of automotive parts, namely the manufacture of General Motor's Safari's step assist (2002), Chevrolet Impala's body side mould (2004) and the H2 Hummer SUV cargo bed (2005), where weight savings of approximately 7-8% were achieved as well as enhancements in mechanical properties compared to their conventional talc filled counterparts. Toyota attributed this to the exfoliated structure obtained within the layered silicate based thermoplastic material. However, there has been relatively little work exploring the incorporation of nanoparticles into thermosetting polymers. Of the work that has been conducted, full exfoliation, or separation of the nanoparticles required for mechanical and fire retardancy property enhancements, has been very difficult to achieve <sup>[2, 3]</sup>, leading this project to investigate the dispersion of nanoparticles in composites to achieve low-cost light-weight materials.

Lowering the resin viscosity during processing increases the potential of polymer molecules to penetrate clay galleries, and is understood to be one of the key factors in facilitating dispersion <sup>[4]</sup>. The rapid (10°C/minute) heating rates achievable using the Quickstep™ process have been shown to lower resin viscosity <sup>[5]</sup>. In addition to this, the mechanical vibration source used with this process aids the separation of clay platelets during the curing process. These features are thought to enable polymer chains to penetrate clay galleries prior to gelation of the polymer, leading to clay separation.

In order to gain an understanding of the optimal degree of clay separation for property enhancement in nanocomposites, characterisation techniques such as XRD, SAXS and TEM were employed.

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## Determination of the structure of a gold based shape memory alloy

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The Au–Cu–Al alloy undergoes a phase transformation which can be tailored for a shape-memory effect, and has been exploited to create sparkling surface patterns in jewellery items. Scientifically-based recommendations for choosing optimal conditions for heat treatment of 18 carat gold pieces in various operations (cutting, soldering, stretching bars) and also under repair conditions have so far been lacking in the jewellery industry. Hence, the objective of this work was to perform *in-situ* powder diffraction at elevated temperatures on the alloy to determine the structure of the material as a function of increasing temperature. Variable temperature powder diffraction has been undertaken at the Australian Synchrotron (10BM1: Powder Diffraction) on spinning 0.3 mm capillaries filled with Au<sub>7</sub>Cu<sub>5</sub>Al<sub>4</sub> powder. In order to solve the crystal structure, determination of the site occupancies was crucial. The synchrotron data are dominated by the scattering length of the Au component. Hence, in order to resolve the site occupancies, complementary room temperature neutron powder diffraction data (with the corresponding change in scattering lengths of the three components) have been collected on Echidna (High Resolution Powder Diffraction) at OPAL, ANSTO. At high temperatures (greater than 630 °C), the Spangold has body-centred cubic packing, with crystal symmetry of primitive cubic. When the temperature falls below 630 °C, a super-lattice forms, which gives satellite peak reflections that can be indexed with face-centred cubic crystal symmetry. Patterns from 630 °C down to 77 °C appear to be face-centred cubic as previously published<sup>[1]</sup>, however there is indication of significant strain in the sample from 290 °C down to 77 °C. Although we are still analysing the data, the indication is that there is more than one phase below 77 °C, and we have detected a previously unknown transition at 50 °C, where the phase composition changes.

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# Neutron reflection study of stimuli-response peptides at the air-water interface

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Biomolecules such as proteins and peptides can self-assemble into well defined structures. The application of self-assembled biomolecules ranges from biomaterials, pharmaceuticals and food, to membrane protein crystallization.<sup>1,2</sup> Recently, a class of rationally designed peptides with the ability to reversibly and precisely control the stability of foams has been developed at the Centre for Biomolecular Engineering (CBE), UQ.<sup>3,4</sup> The air-water interfacial structure of two peptides, AM1 and Lac21, have been investigated by neutron reflectometry.<sup>5</sup> We have partially deuterated these peptides and conducted measurements at 6 different contrast conditions (deuterated and non-deuterated samples at a varied ratio of H<sub>2</sub>O/D<sub>2</sub>O), in order to determine interfacial distribution profile of peptide molecules. The results show that there is a clear separation between hydrophobic and hydrophilic sub-layers of the peptides (ca. 7.5 Å for AM1 and ca. 6 Å for Lac21E), a key feature of an  $\alpha$ -helix structure of the peptides. Furthermore, we revealed that AM1 can drastically change its mechanical properties without altering its surface population while Lac21E switching is based on peptide dissociation at the interface.

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