

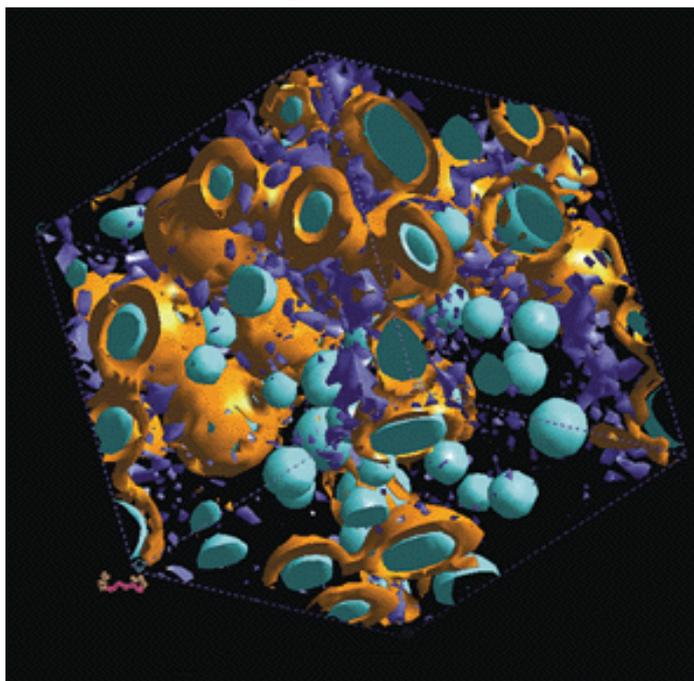
Materials Monthly

Volume I, Issue 5

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Centre for Science and Engineering of Materials

Modeling Materials



Phase separation in a polymer blend, computed using the mesoscale modeling methods of Mesodyn.
<http://www.mathub.com/gallery/polymers.html>

"The time has passed when molecular modeling was viewed as 'just a lot of pretty pictures'.

The convincing scientific and business evidence that supports the value of molecular modeling has persuaded all but the most die-hard anti-modelers that modeling translates to real science and real business.

Having won that battle, some modelers are now fighting on another front - to have modeling accepted as art."

Mat Hub, www.mathub.com

The new site, Mat Hub, is a focal point for computational materials science on the web, providing a gateway to scientific information about modeling and informatics. It was launched in February this year by Molecular Simulations Inc.

What is Materials Modeling?

According to Mat Hub: *Materials modeling is the application of computational and modeling techniques to characterize the structure and predict the*

properties of solid state and molecular systems.

Since the macroscopic properties of materials are controlled by their microscopic behaviour, materials science software can assist in the design and analysis of all types of materials. Modeling software enables you to analyze the structure of materials from the sub-atomic scale, through the atomic and molecular scale, to the mesoscale, and to analyze their chemical properties.

At the ANU, a significant number of scientists in many fields, are using materials modeling as an integral part of their research. For example, materials science in Engineering, Chemistry and Applied Maths relies heavily on computational modeling techniques.

To help make up your own mind about the 'science or art?' issue, check out examples of modeling used in the world of art via the *Molecular Gallery*: www.mathub.com/gallery/index.html

What's Inside

- 2 Direct from the Director
- 3 GeoMaterials on Campus: Petrophysics
- 4 Jobs & Scholarships For your diary
- 5 Photonics Education
- 6 Communication Contacts



Direct from the Director

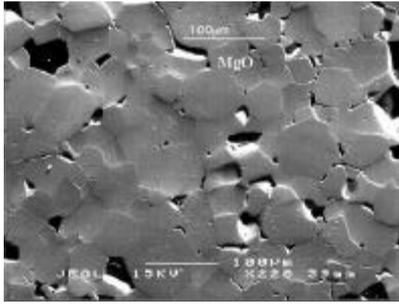
Phil Evans, Forestry Department

Contact with industry is becoming increasingly important in gaining access to government funds for research. Indeed for many schemes, evidence of industry collaboration (in-kind and cash support) is a prerequisite for gaining access to grant monies. In Canberra we suffer from the disadvantage that we are isolated from many of the industries that could provide the necessary assistance, which may, in part, account for the ANU's relatively poor record in this year's SPIRT round, where we obtained 4 grants compared to 52 and 44 for UNSW and U. Melbourne, respectively.

At the moment I am organising the 5th Pacific Rim Biobased Composites Symposium, which will bring over 200 delegates to Canberra in December (10-13th, see <http://www.anu.edu.au/Forestry/wood/bio/bio.html> for further details). The symposium has attracted considerable numbers of people from industry as well as scientists from most countries in the region. The following companies will be represented at the symposium; Orica Adhesives and Resins; Bondtite; Borden Chemicals; Huntsman Chemical Company; Taranaki Nuchem; Krens Chemie (Austria); Dominance Industries; Fletcher Wood Panels (New Zealand); Laminex; Fentak; Mitsui Wood Systems (Japan); U.S. Borax; Siempelkamp; Yamahah Corporation (Japan); Stephen Young & Assoc; Carter Holt Harvey; Starwood; Pyropanel Technologies; Olsen and Vickery; Dyno Industries (Singapore).

For those of you with interests in resins, adhesives (particularly emulsions) biocides, structural engineering, composites (structure v function) and analytical chemistry, the symposium represents a good opportunity to make contact with industry and find out what their research priorities are likely to be in the coming years. If you would like an opportunity to meet with the industry people coming to the symposium (the dinner will be held at Parliament House on 13th of December) then please get in contact with CSEM (CSEM@anu.edu.au).

Geomaterials on Campus:



Research School of Earth Sciences

Petrophysics Group

The research activities of the Petrophysics group focus on experimental studies of the mechanical properties of rocks and minerals with application to fields of seismology, structural geology, geodynamics and materials science. Analysis of crystal defects and microstructures in rocks and minerals by both light and electron microscopy, and comparison of laboratory work with data and materials collected in field-based programs, are essential aspects of many of the research activities. Specialised equipment provides a unique facility for experimental investigation of the elastic, anelastic, plastic and brittle behaviour of materials at high pressures and temperatures.

Specific areas of current interest include:

Seismic Properties

- The study of physical properties of rocks and minerals under lab-conditions which simulate those within the Earth - with particular emphasis on the measurement of elastic wave speeds and attenuation under conditions of high pressure, pore pressure and temperature; the application of similar experimental methods in the characterisation of non-geological materials such as ceramics and metals;
- the interpretation of the observed behaviour in terms of the fundamental physics and chemistry of crystalline and partially molten materials, and fluid-saturated porous media;
- the application of well-understood laboratory data in the interpretation of seismological models for the spatial variation of density, elastic wave speeds and attenuation;
- analysis of the constraints imposed by such interpretation upon the constitution and evolution of the Earth.

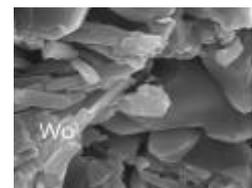
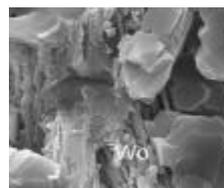
For more info see: ses.anu.edu.au/rockphysics

Rock Deformation/Fluid Interaction

Experimental investigations focus on the mechanical behaviour and fluid transport properties of rocks in high temperature environments where the presence of fluids influences strength and deformation processes. One goal of this work is to refine our understanding of earthquake mechanics and fluid transport in active fault zones where fluid-rock interaction is important in controlling earthquake nucleation and recurrence. The experimental program is also investigating the effects of fluid-driven reactions on the evolution of permeability and strength in rocks undergoing phase changes in high temperature crustal regimes.

The experimental studies are complemented by field-based investigations which examine -

- how fluid pressure fluctuations, fluid mixing and fluid-rock interaction influence the dynamics of ore deposition in tectonically active settings.
- the role fault/fracture/shear zone connectivity plays in controlling the architecture of fluid flow and distribution and timing of ore genesis during crustal deformation.



Microstructures

Experimental investigation of the distribution of basaltic melt in rocks similar to those of the Earth's upper mantle, with the aim of constraining the melting processes at mid-ocean ridges, subduction zones and hot-spots (e.g. Hawaii). Samples are synthesized at upper mantle pressures and temperatures and examined with a range of electron microscopy techniques. One of our interests is how deformation and the resulting preferred orientation of the crystalline grains affects grain boundary structure and melt distribution, where grain orientations can be mapped by electron-backscattered diffraction. Other projects include direct permeability measurements on texturally equilibrated analogue materials such as marble, and comparison of pore shapes with the shapes of melt "pockets" in partially molten rocks.

Jobs & Scholarships

ANU

University House Accommodation Scholarship

Uni House will again offer a scholarship, of one year's free accommodation, to be held by a doctoral student currently enrolled at the University. Applications are invited with a closing date of Friday 24 November, and the scholarship will be available from January.

Contact Gail Reekie of the Graduate School on x5922 or email: Graduate.School@anu.edu.au for further information.

Complex Materials Studies - Research Fellow/Fellow

Applied Maths, RSPHYSSE

Further info: rshysse.anu.edu.au/appmaths or Stephen.Hyde@anu.edu.au

Theoretical Plasma Physics - Postdoc/Research Fellow

Physics and Plasma Research Lab, RSPHYSSE

Further info: rshysse.anu.edu.au/~rld105 or robert.dewar@anu.edu.au

Experimental Chemical Physics - Postdoc/Research Fellow

Atomic and Molecular Physics Lab, RSPHYSSE

Further info: rshysse.anu.edu.au/ampl or brenton.lewis@anu.edu.au

Atom Optics, Nanotechnology, Atomic Collisions - Research Fellow/Fellow

Atomic and Molecular Physics Lab, RSPHYSSE

Further info: rshysse.anu.edu.au/ampl or stephen.buckman@anu.edu.au

Australia

Prime Minister's Prize for Science

Malcolm McIntosh Prize for Achievement in the Physical Sciences

You are invited to consider making nominations for these prizes.

Nomination information is available at www.isr.gov.au/science/

Overseas

*Just a few of the 44 MSE jobs listed at jobs.ac.uk

*Lectureships/Readerships in Chemistry and Physics

Departments of Chemistry and Physics - **University of Southampton**

*Research Fellow in Photonic Crystal Circuits

Department of Electronics and Computer Science & Optoelectronics Research Centre - **University of Southampton**

***PhD Studentship: Molecular Recognition in Robust Imprinted Polymers and Biomimetic Metal Nanoparticles**
Department of Chemistry - **University of Liverpool**

***Assistant Director of Research Experimental Surface Science**
Department of Chemistry - **University of Cambridge**

***PhD Studentship: Environmentally Assisted Cracking of High Strength Aerospace Steels**

Department of Materials Engineering - **University of Wales, Swansea**

***Postdoctoral Position Multiaxial Creep/Fatigue of polycrystalline Nickel-base Superalloys**

Department of Materials Science and Metallurgy - **University of Cambridge**

***Postdoctoral Research Assistant (two posts) Electrodeposited Semiconductor/Materials and Devices for Light Emitting and Solar Cell Applications**

Applied Physics Division - **Sheffield Hallam University**

***Postdoctoral Research Associateships and PhD Studentships Physics and Application of Molecular Materials.**

The Blackett Laboratory & Centre for Electronic Materials and Devices - **Imperial College of Science, Technology & Medicine**

***Post-Doc/Research Fellow : Theoretical Polymer Scientist.**

Theoretical and computational prediction of the properties of dental biomaterials. IRC in Biomedical Materials and Centre for Computational Science - Queen Mary and Westfield College, **University of London**

Two Research Fellowships for Women in Science, Mathematics or Engineering

Newnham College Cambridge. More info: The Principal's Secretary, Newnham College, Cambridge CB3 9DF

Research Fellowships in Physical Chemistry, Engineering, Metallurgy or Physics

University of Oxford. More info: www.admin.ox.ac.uk/fp/

Head of Wood Science Department

University of British Columbia. More info: Dr Bart Van der Kamp, vdkamp@interchg.ubc.ca

For Your Diary

- **Australia New Zealand Forensic Science Society ACT Branch Seminar** Nov 28
The Canberra Mail Centre Bombing: Presented by Federal Agent Tom Stoewer, Australian Federal Police Forensic Services Unit, at 7.30pm in the Canberra Hospital Auditorium. Cost \$10/\$5, bookings essential: clifton.frost@afp.gov.au, ph 6287 0396
- **"Atomic Scale Materials Characterisation with Synchrotron Radiation"** Nov 29
CSEM seminar presented by Mark Ridgway, Electronic Engineering Materials Department, RSPHYSSE at 4pm in the seminar room on the first floor of the Link Building (# 58D, joins the Cockcroft and Oliphant Buildings). Followed by drinks and nibbles across the hall.
- **Australian Composite Structures Society Seminar** Dec 4
Dr Jonathan Hodgkin, CSIRO Molecular Science will present a seminar from 4-5pm in the Ian Ross Building (#31, Dept of Engineering) Seminar Room. More info: bronwyn.fox@anu.edu.au
- **The "New" ARC Grant Schemes - Information Seminar** Dec 6
1.30pm in the Haydon Allen Tank. Bookings essential, phone x0099 or email Reserach.Services.Office@anu.edu.au
- **5th Pacific Rim Bio-Based Composites Symposium** Dec 10-13
hosted by ANU at Rydges Canberra Hotel, Canberra. More info: Phil.Evans@anu.edu.au
- **Raman Microscopy Workshop** Feb 2000
Presented for CSEM by Vincent Otieno-Alego of the University of Canberra's Microscopy Unit for Materials Analysis. Contact Phil.Evans@anu.edu.au for more info.

Photonics Education:

light at the end of the tunnel



Did you know? *The largest private employer in the ACT is ADC Australia, a photonics fibre components manufacturer. The company already employs more than 400 staff.*

On Wednesday 8th November, I represented CSEM at a Photonics Education Forum organised by the Australian Photonics Cooperative Research Centre and the Australian Electrical and Electronic Manufacturer's Association (AEEMA). Several other CSEM members, more directly involved in the photonics field, were also present. Attended by researchers and educators, industry professionals, communicators and senior government representatives; the aim of the forum was to report on and discuss photonics outreach, course development and delivery, and the development of skills relevant to the industry.

It is forecast that at current levels of photonics education and training, Australia will soon have a massive shortage of suitably qualified people to fill the thousands of positions to be generated by this rapidly emerging industry.

Of local interest is the plan by ANU to offer two new undergraduate degrees for 2002: a B.Sc (Photonics) and a B.E. (Photonic Systems). These specialist degrees have been made possible by funding from the VC's Plan for Growth initiative and are expected to gain additional ongoing support from industry partners. The final year of each degree will be taught largely by active photonics researchers (locally from the Department of Physics and Research Schools of Physical Sciences and Engineering, and Information Sciences and Engineering). This arrangement will provide students with an insight into the very latest developments in this highly technological and innovative field. Photonics fits well under CSEM's cross-disciplinary umbrella (via the Optical and Electrical Materials category) and the Centre intends to support these new courses in the form of cross promotion and further collaboration.

Also announced at the conference was the signing of a major contract between the CRC and Questacon—The National Science and Technology Centre—regarding the promotion of photonics technology and careers to senior high school students across Australia via the traveling Shell Questacon Science Circus. The presenters of this highly acclaimed national outreach program are science graduates, simultaneously undertaking the ANU Graduate Diploma in Scientific Communication.



What is photonics? *The generation and harnessing of light: emission, transmission, amplification and detection; lasers; fibre optics, electro-optical instrumentation, related electronics, and sophisticated systems. The range of applications of photonics extends from energy generation to communications and information processing.*

The information technology (IT) industry that has captivated the government and community and is seen by many as the way to a prosperous future, is built upon photonics technology. Photonics enables us to communicate, access and process information so rapidly (and increasingly so). Unlike the IT industry, the photonics industry develops and manufactures most of its hardware in Australia and exports large quantities of photonics components overseas (as much as 90%). Australia is emerging as a competitive force on the world market in the production and export of a wide variety of photonics components, devices and systems. While the Australian IT industry may be employing large numbers of people, it does not make its own computers or export large amounts of product.

The emerging photonics industry deserves strong support, however, it was obvious from the forum that key players need to dedicate more time to lobbying and educating our government about its relevance and potential.

Jenny Edwards

Career opportunities: *The exponential growth in the photonics industry worldwide means that there are excellent career opportunities both in Australia and overseas. An increasing number of start-up companies in photonics are appearing across Australia, and some larger existing companies are rapidly expanding their photonics activities. Following a recent survey, it has been estimated that Australia will need some 24,000 people in the photonics industry by 2010, predominantly with either TAFE or university level training in photonics and related disciplines. Already there are a number of young Australian millionaires who joined such companies within the last decade and benefited from their stock-option schemes.*

The Photonics Education Forum was followed by an Industry Forum on Thursday 9th November. For further information contact:

Prof Mark Sceats, CEO Australian Photonics CRC
Tel: +61 2 9351 1909/1901
Fax: +61 2 9351 1910
Email: info@photonics.crc.org.au

Prof John Love, Optical Sciences Centre, RSPHysSE, ANU
Tel: +61 2 6249 4691
Fax: +61 2 6279 8588
Email: jdl124@rsphysse.anu.edu.au

or view: www.photonics.crc.org.au/

Communication News

CSEM Seminar: "Atomic Scale Materials Characterisation with Synchrotron Radiation" - Mark Ridgway of the Electronic Engineering Materials Department, RSPHysSE will be presenting the above seminar on Wednesday 29 November at 4pm in the seminar room on the first floor of the Link Building (# 58D, joins the Cockroft and Oliphant Buildings). Followed by drinks and nibbles across the hall.

CSEM Consultative Committee Meeting - the committee will be meeting on Thursday 30 November to review recent CSEM activities, comment upon the proofs of our new promotional materials and discuss future directions.

ANU Materials Science attracts Large ARC Grants - congratulations to the ANU materials scientists involved.

- Formation mechanism of boron nitride nanotubes produced by reactive ball milling
Dr Ying Chen - Dept of Engineering/RSPHysSE, Prof Jim Williams - RSPHysSE, Dr John Fitzgerald - RSES
- Advanced organometallic materials
Dr Mark Humphrey - Dept of Chemistry, Dr Marek Samoc - RSPHysSE, Dr Graham Heath - RSC
- 3D to 4D architecture of fluid flow in fault and shear zone networks during crustal deformation
Prof Stephen Cox - Dept of Geology/RSES

For more info on successful Large ARC Grant Scheme applications see: www.arc.gov.au/grants/outcomes

CSEM

Centre for Science and Engineering of Materials

Faculties

Department of Chemistry
Department of Engineering
Department of Forestry
Department of Geology
Department of Physics

Institute of Advanced Studies

Research School of Biological Sciences
Research School of Chemistry
Research School of Earth Sciences
John Curtin School of Medical Research
Research School of Physical Sciences and Engineering

Institute of the Arts

Materials Workshops

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We welcome any feedback, enquiries or contributions.

Please let us know if you wish to be added to our electronic or postal mailing lists.

Electronic copies of *Materials Monthly* can be accessed at:

www.anu.edu.au/CSEM