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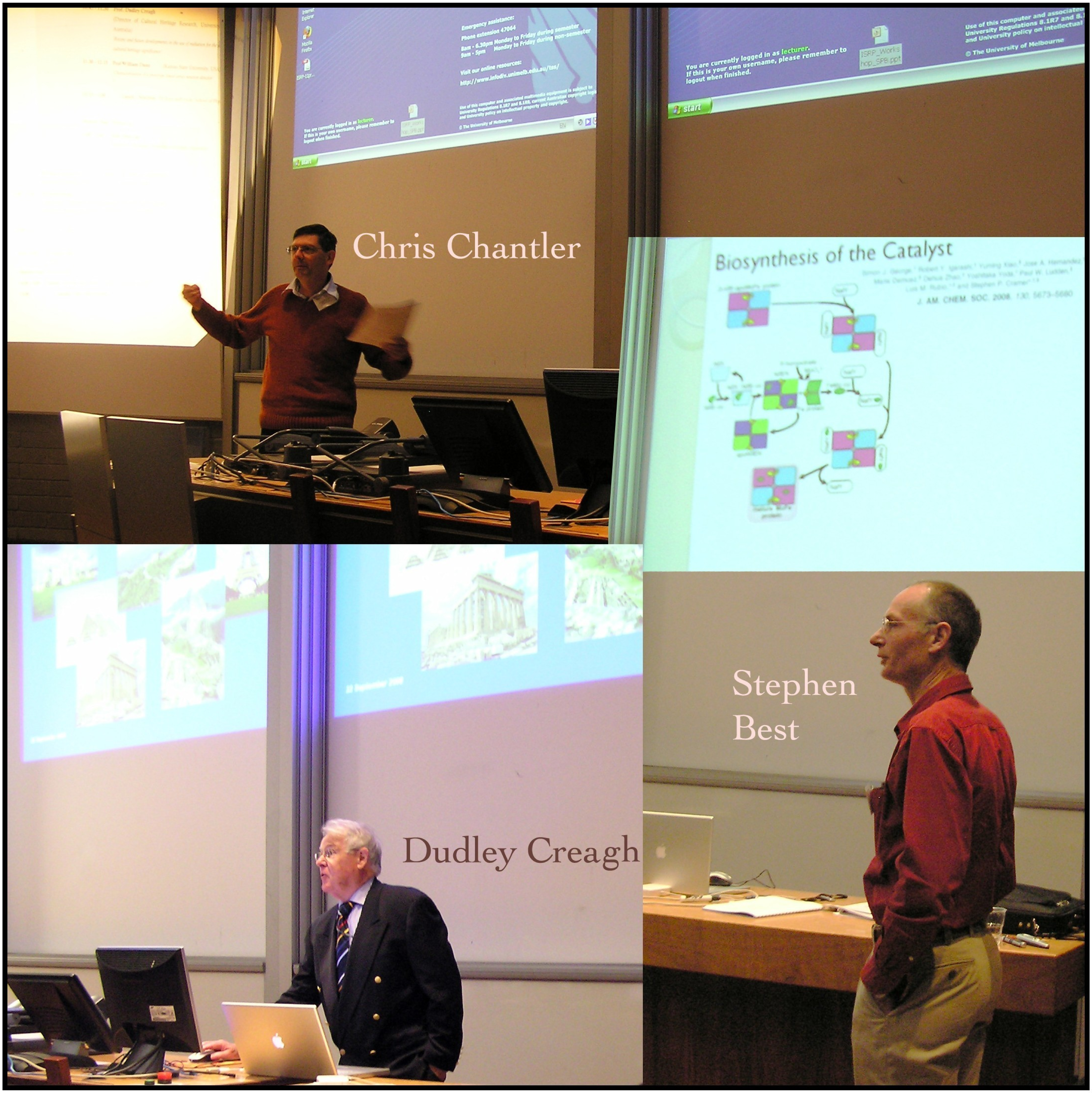

The Australians (some pictured above) were in full force at the recent International Forum on Future Directions in Atomic and Condensed Matter Research and Applications (22 and 23 September 2008, School of Physics, University of Melbourne).
Sponsored by IRPS, the Australian Synchrotron, the University of Melbourne, and the State of Victoria, the program is reproduced via this button.
Photos : Larry Hudson

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FROM THE EDITORS

Greetings all and welcome to the 3rd issue of the IRPS Bulletin for 2008. When last you heard from us the sun was poised over the northern tropic, and the image of our spinning planet beneath evoked something of the common purpose that animates our international community peacefully pursuing initiatives in radiation physics. Since then, our orbit has carried us around to an intermediate point, between equinox and solstice, where the tumult of seasonal change has been echoed by upheavals in global financial markets that have exposed fault lines in the economic foundations upon which many of these same initiatives, if not our host institutions and, perhaps, personal livelihoods, may depend.

The international scope of these developments is breathtaking, but equally so is the complex interplay of local and more broadly regional efforts to plug the leaks and to engineer a new regulatory regime from the ashes. From our present vantage point, the consequences of the market meltdown for our individual research enterprises may be difficult to predict, but by staying in touch and sharing our success stories as well as our failures, we all stand to benefit from a uniquely diverse set of perspectives.

Here at the IRPS Bulletin, the series of reports from regional Vice Presidents has provided something of that perspective. The present issue continues our series with a report from Bill Dunn that brings us up to date on certain issues and activities – and meteorological hazards – impacting radiation physics in the USA. We are also pleased to reprint abstracts from the recent International Forum on Future Directions in Atomic and Condensed Matter Research and Applications, held in Melbourne, Australia in September. Upon the announcement of John Hubbell's death last year, many of you sent your condolences and wishes for his widow, Jean, so you'll be pleased to know that we have recent pictures of her accepting the JARI Medal, awarded posthumously to John at the annual meeting of the Council on Ionizing Radiation and Measurements Science, held at NIST (USA) in October.

Finally, the unpredictable changes wrought by climate and market forces stand in stark contrast to the type of change occasioned by elections. With the triennial election of IRPS officers just around the corner, we also have published a preliminary slate of candidates for you to consider and, perhaps, augment. We echo the sentiments of our President in urging your participation in this election and the activities of the IRPS. Let us hear from you so that we may share your stories and continue to learn from one another.

Ron Tosh and Larry Hudson

PRESIDENT 'S REPORT

The recent decision at its Congress in Osaka, Japan (2008) by the International Union of Crystallography to create a Commission on Crystallography in Art and Cultural Heritage underscores the fact that art and cultural heritage is considered to be of significance. And that there is a real need to encourage the growth of the field of conservation science so that we may better conserve and preserve artefacts and buildings which society considers of significance
to it.

What is considered to constitute art and cultural heritage varies from person to person, community to community, and nation to nation. Cultural heritage may be seen by many as large monuments of historical significance: Stonehenge in England, the Pyramids of Egypt, the Parthenon in Athens, the Great Wall of China, Ankor Wat in Cambodia, the tombs in the Valley of the Kings in Korea, Machu Picchu in Peru, and so on. But to others more simple structures may have resonance: cave paintings of, say, the indigenous Australians, a simple wooden building in Australian Antarctica (Mawson's Hut), wooden churches in Russian Siberia, for example.

And what is considered to be art has elements which stretch from cave paintings drawn 4000 years ago, through the classical European painters, to impressionists, to cubists, to post-modernists, and so on. And art is not simply a collection of paintings. It encompasses everything devised by man for the enhancement and embellishment of his environment. Basic items such as bowls, jugs, cutlery, jewelry, swords, spears, and chariots all can be viewed as art. In the archaeological context we often know nothing about cultures which have flourished in the past except through their art: there was no written language. So all that is left of those cultures are items of art, work, and war which have been associated with a burial, or have been covered by some man-made or natural disaster.

Both art and cultural heritage tell us where we have come from, and who we now are. Emotionally cultural heritage is important to us. Some heads of nations have sought to destroy the past, change the record of history, and redirect the way we think. Think of Pol Pot in Cambodia, or for that matter, successive Pharaohs in Ancient Egypt.

But art and cultural heritage are big business. Many nations survive economically on their wealth of cultural heritage. If their patrimony is not adequately protected these countries will suffer significant financial loss. Established nations and national groupings have the means, the intellectual property, and the will to protect their art and cultural heritage. Now the International Union of Crystallography has affirmed its recognition that there is a need to have an **international** emphasis in the field on Scientific Conservation. In this they join another United Nations sponsored body, the International Council of Museums. There is a desperate need for these bodies to help less advanced nations to preserve their own art and cultural heritage through training and direct practical project assistance.

As you know, our Society has, in recent years, been engaging in a small way, the development of scientific initiatives in the field of cultural heritage conservation. And at ISRP-11 the associated workshop will offer lectures on scientific conservation and on the basic skills needed by conservators.

Cultural heritage is not simply a matter of things, buildings, and monuments. It is created by people. People, and their involvement in all aspects of living, create cultural heritage.

In this Bulletin we seek your involvement in the life of our Society by being part of the election process for the next IRPS Council. This issue will contain suggestions by the IRPS Council as to the membership of the future Council. If you wish to nominate for the Council, please contact the Secretary to find the mechanism for doing so.

The active involvement of members is essential for the continuing health of all societies.

Dudley Creagh

Vice President's Report, North America

William L. Dunn

Department of Mechanical and Nuclear Engineering, Kansas State University, 346 Rathbone Hall, Manhattan KS 66506-5205

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The most important item with which I can open this report is the sad news that our colleague and dear friend John Hubbell passed away within the last year. John helped in the formation and maturation of IRPS and served for many years in various offices of the Society. He and his lovely wife Jean were fixtures at all of the Symposia organized by the Society through the last one in Coimbra. On a personal note, I will remember John as an indefatigable worker, whose papers we have all referenced many times, and as both an accomplished scientist and a wonderful person. His work was his life, in the sense that he was devoted to radiation physics and could not retire fully from it. Yet he also was devoted to his wife and family. The radiation physics community and this Society will sorely miss our dear colleague John Hubbell.

On other matters, there is encouraging news from North America. The broad area of nuclear science and engineering is seeing a renaissance in the US, which mirrors that seen in many other continents around the world. This is based primarily on the anticipated resumption of the construction of new nuclear powerplants in the US, which in itself has little to do with radiation physics. However, the acceptance by society that nuclear energy is a valuable option in addressing our growing energy needs leads to the general perception that nuclear energy (and by association radiation) is our friend. As I reported in a previous newsletter, this fact has led to a tremendous growth in students seeking nuclear training. This can only bode well for those of us who teach and work in the basic and applied radiation physics fields.

I will be somewhat colloquial in my few next statements, but these are things with which I am familiar. First, the TRIGA reactor at Kansas State University (KSU), where I am employed, has received its license to increase power to 1.25 MW. The core has been reconfigured and operation above 0.75 MW has been achieved.

This is noteworthy because it reverses a trend. Many research reactors in the US have been closed and decommissioned over the last several decades. The licensing of our research reactor for a five-fold increase in power hopefully will reverse that trend. Second, the Spallation Neutron Source (SNS) is going through extensive operational testing and will soon be offering its beam lines to scientists around the world. A prototype linear-array neutron detector developed at KSU has been delivered to SNS for testing. A 1000-channel array with approximately 100-mm pitch is being developed for delivery next year. Third, The KSU TRIGA reactor building was directly hit, on 11 June 2008, by a tornado, which inflicted over $20 M damage to the KSU campus. The tornado ripped off many of the roofing panels over the reactor bay, but there was no real structural damage to the building or the reactor. The debris that was deposited in the pool of the reactor has been removed, a temporary roof has been installed over the reactor, and a new roof has been pledged to be installed by mid-August, when students will return for the fall semester. The fact that the reactor facility had been designed and constructed so well as to be able to withstand the potentially devastating effects of a direct tornado strike is reassuring not only to those of us in the broad research community but also to those in the local community.

Finally, I wish to mention that the seventh Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications (IRRMA-7) was held in Prague, Czech Republic, from 22-27 June 2008. Over 150 attendees were treated to good science at the meeting and delightful sights and experiences in the beautiful city of Prague. Ladislav Musilek, a member of the IRPS council, is to be heartily congratulated for organizing and hosting the IRRMA-7 conference. Several IRPS members including President Dudley Creagh, Secretary David Bradley, and Vice President Jorge Fernández—were in attendance. Also, I announced at the meeting that IRRMA-8 will be held in Kansas City, MO, from 26 June to 1 July, 2011. I hope that many of you will plan to attend this meeting, which is closely aligned with the interests of IRPS.

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John Hubbell is Awarded the JARI Medal posthumously

received by his widow, Jean Hubbell

Testimonial from Stephen Seltzer, N.I.S.T

As you all know, John Hubbell was a physicist and former member of the Ionizing Radiation Division here at NIST. In 1950 he came to work at the National Bureau of Standards (NBS) in Washington, D.C.; he retired in 1988, but worked full-time continuously as a Guest Researcher until March, 2007, when he had a stroke, leading to his death at 81.

John's career essentially started in the Radiation Theory Section, headed by Ugo Fano. His other colleagues in the Section included Martin Berger, Lew Spencer, Herb Attix, Haaken Olsen, Kjell Mork, Lenny Maximon, and of course many others. I joined the Section in 1962 and am proud to have had John as valued colleague, lunch buddy and friend until his death.

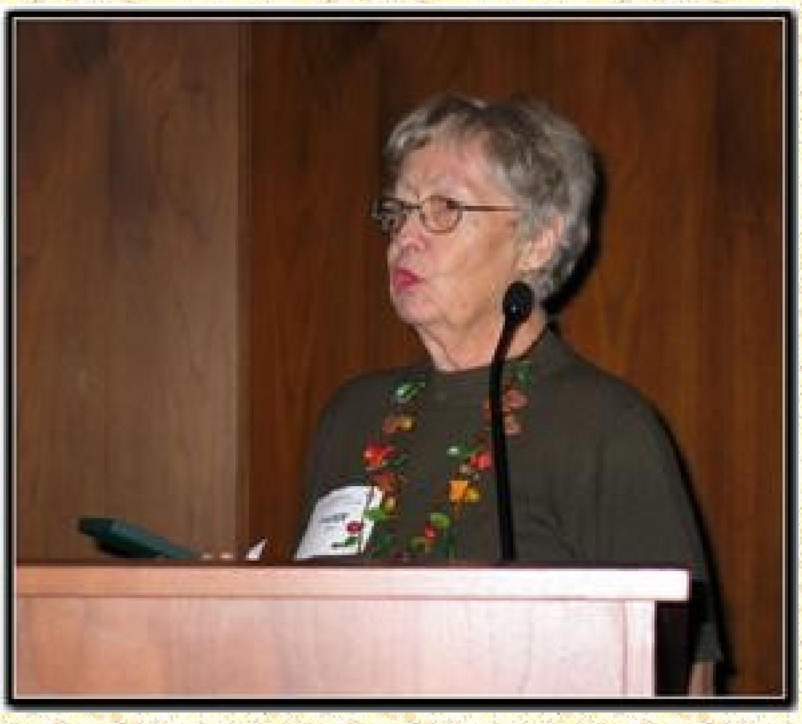
John was the world leader in providing critically evaluated standard reference data on x-ray and gamma-ray interactions with matter. He proposed the formation of the X-Ray and Ionizing Radiation Data Center (now known as the Photon and Charged-Particle Data Center) to better our understanding of photon-interaction phenomena and to provide the most accurate data available. He was Director of this Center from 1963 to 1981. I became Director in 1988 (Martin Berger had it in between), but John largely kept it going even as a Guest Researcher.

John was an indefatigable correspondent, mentor, and world-traveler. A hallmark of John's was to attract the world's other experts as collaborators; and this international involvement in physics led him to co-found, with Dick Pratt, the International Radiation Physics Society in 1985. He also became Editor of ***Applied Radiation and Isotopes***, and Editor-in-Chief of ***Radiation, Physics and Chemistry***.

He served as Vice-President and President of the International Radiation Physics Society. He was a Fellow of the American Nuclear Society, of the Health Physics Society, and of the American Physical Society; a member of the Radiation Research Society and the Society of Nuclear Medicine. He served on numerous committees of these societies and was a consultant to the International Commission on Radiation Units and Measurements, the International Union of Crystallography, and the World Health Organization/IAEA.

He received honors too numerous to mention here, including, of course, this JARI award. But I think instead that it was John who honored us. Not just his family and friends who knew him personally, but all of you attending this meeting, your colleagues, and your students. For I have no doubt that every one of you here, indeed nearly everyone in radiation physics, depends on his data for their work. That you can take it for granted is due to his work and accomplishments.

Thank you



In addition to the plaque that Jean will take home, I want to add my thanks to John and his work. Please stand and join me in a moment of silence in tribute to John Hubbell.

IRPS Council Meeting

The IRPS Council meeting followed on from the International Forum, on 25 September, also at the University of Melbourne and hosted by Chris Chantler.

Participants :

Lower photo - standing left to right :
William Dunn, Shirley McKeown, Chris Chantler, Isabel Lopes, Jorge Fernandez, Rex Keddy

Seated left to right :
Richard Pratt, David Bradley, Dudley Creagh (IRPS President), Malcolm Cooper, Larry Hudson.

Photos : Larry Hudson

The next council meeting is scheduled for 23 April 2009 at Guildford, UK and will be hosted by David Bradley.

International Forum on Future Directions in Atomic and Condensed Matter Research and Applications

Chris Chantler,
Associate Professor and Reader
School of Physics, University of Melbourne, Melbourne, Australia

Following are the Introduction, Programme and Abstracts from this Forum which took place on 22nd and 23rd September, 2008, at the University of Melbourne, Melbourne, Australia.

Supporting Organisations were :

Endorsed by the IUCr International Commission on XAFS

I hope you find this Forum to be interesting and useful to show links between some of the key threads across disciplines from Physics and Chemistry through Synchrotron Science, Diffraction, Biophysics, Biomedicine and Engineering. The Forum begins with experts on the fundamental side in theory and experiment and leads towards diverse critical applications, finishing off with a forum to discuss key recent advances, personnel and possible future linkages and efforts. The thread of Atomic and Condensed Matter theory and Science is crucial to several developing applications and opportunities across these fields, and this is a key focus. This is a Forum coordinated by the International Radiation Physics Society and by the School of Physics, University of Melbourne. We are gratefully supported by DEST in part as a coordination and communication opportunity and in part as a preparation for the International Symposium on Radiation Physics – 11 in Melbourne September of next year 2009. We are gratefully supported by the Australian Synchrotron for direct relevance to existing and up-coming opportunities in synchrotron research and applications. And we are gratefully endorsed by the IUCr International Commission on XAFS (X-ray Absorption Fine Structure) for the development of links & teaching with the wider community. I feel that we will attain all of these objectives. The Invited Plenaries are also invited to contribute field and forward-looking reviews in their respective areas to a special issue of the Radiation Physics and Chemistry journal. This will undoubtedly develop and extend some of the ideas presented in the Forum. I hope that in all several strengths and key opportunities are shown in the Forum, but the readers and attendees will be the judges of that! My acknowledgements and thanks to all international and national Speakers, Session Chairs, and attendees, and especially to Justin Kimpton (Secretary) and Stephen Best (Chemistry) and my students for their assistance in preparing the program. Very best wishes and welcome.

../Programme

International Forum on Future Directions in Atomic and Condensed Matter Research and Applications

Hercus Theatre, Physics, University of Melbourne

22nd & 23rd September, 2008.

Supported by the Australian Synchrotron, DEST, IRPS & University of Melbourne

All welcome. There are no registration fees. A tea/light lunch will be provided. Please indicate special dietary requirements. To estimate numbers and for book of abstracts please email to Dr. Justin Kimpton (jkimpton@unimelb.edu.au) by Monday 8th September, 2008

Programme

Monday

9.00 - 9.10	**Opening: Deputy Vice-Chancellor (I), University of Melbourne, Prof. Frank Larkins**
9.10 - 9.15	**Prof. Liz Sonenberg, Dean of Science, University of Melbourne**
9.15 - 10.00	**Prof. Richard Pratt** (University of Pittsburgh, USA) *'Compton scattering revisited'*
10.00 - 10.45	**Prof. Malcolm Cooper** (University of Warwick, UK) *'Resonant X-ray diffraction studies of magnetism'*
10.45 - 11.00	**Tea / Coffee**
11.00 - 11.45	**Dr Isabel Lopez** (University of Coimbra, Portugal) *'Condensed noble gases for direct dark matter search'*
11.45 - 12.30	**Dr Larry Hudson** (National Institute of Standards and Technology, USA) *'Laser-produced X-ray sources'*
12.30 - 1.15	**Lunch / Selection & posters** 7th floor staff room, School of Physics
1.15 - 2.00	**Dr Jorge Fernandez** (University of Bologna, Italy) *Characteristic X-ray spectra: Developments in understanding, status and future opportunities'*
2.00 - 2.45	**Prof. Marcelo Rubio** (Universidad Nacional de Cordoba, Argentina) *'Latest developments and opportunities for 3D analysis of biological samples by confocal micro-XRF'*
2.45 - 3.00	**Tea / Coffee**
3.00 - 3.45	**Prof. Rob Lamb** (Director of the Australian Synchrotron, Australia) *'Major scientific developments at synchrotrons and at the Australian Synchrotron, and prospects for future directions'*
3.45 - 4.30	**Prof. Joel Brugger** (University of South Australia) *'Synchrotron-based techniques in mineral exploration'*
4.30 - 5.15	**Prof. Andris Stelbovics** (Director CAMS, Curtin University, Western Australia) *'Reflections on eighty years of progress in electron-atom scattering '*
5.15	**Monday Close**

../Tuesday

International Forum on Future Directions in Atomic and Condensed Matter Research and Applications

Tuesday

9.00 - 9:45	**Assoc. Prof. C. T. Chantler** (University of Melbourne, Australia) *'Accurate measurement and physical insight: The X-ray Extended Range Technique for fundamental atomic physics, condensed matter research and biological sciences'*
9.45 - 10.30	**Prof. Peter Colman** (Walter Eliza Hall Institute, Australia) *'Crystallography without crystals'*
10.30 - 10.45	**Tea/Coffee**
10.45 - 11.30	**Prof. Dudley Creagh** (Director of Cultural Heritage Research, University of Canberra, Australia) *'Recent and future developments in the use of radiation for the study of objects of cultural heritage significance'*
11.30 - 12.15	**Prof William Dunn,** Kansas State University, USA *'Characterization of a prototype linear array neutron detector'*
12.15 – 1.00	**Lunch / Selection,** 7th floor staff room, School of Physics
1.00 – 1.45	**Prof. Peter Lay** (School of Chemistry, University of Sydney, Australia) *'Biomedical applications Of X-Ray absorption and vibrational spectroscopic microscopy in obtaining structural information from complex systems'*
1.45 – 2.30	**Dr David Bradley** (University of Surrey, UK) *'Applications of condensed matter understanding to medical issues and disease progression: Elemental analysis and structural integrity of tissue scaffolds'*
2.30 - 3.15	**Tea/Coffee**
3.15 – 4.00	**Dr Stephen Best** (School of Chemistry, Melbourne) *'Application of XAFS to biologically-relevant metal-based chemistry'*
4.00 – 5.00	**Forum** - most innovative papers / authors /research since 2000
5.00	**Tuesday Close, End of Forum**

../Abstracts

Compton Scattering Revisited

R. H. Pratt

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA

We review the standard theory of Compton scattering from bound electrons, and we describe recent discoveries that require modification of the theory, noting the nature of consequences for experiment. The subject began with Compton scattering from free electrons. Experiment actually involved bound electrons, and this was accommodated with the use of impulse approximation (IA), which described inelastic scattering from bound electrons in terms of scattering from free electrons. This was good for the Compton peak, but failed for soft final photons. The standard theory was formalized by Eisenberger and Platzman (EP), whose work also suggested why impulse approximation was better than one would expect, for doubly differential cross sections, but not for triply differential cross sections. Relativistic modifications of IA were worked out by Ribberfors. And Bergstrom and Suric developed a full relativistic second order S matrix treatment, not making impulse approximation, but within independent particle approximation (IPA).

Newer developments in the theory of Compton scattering include: (1) Demonstration that the EP estimates of the validity of IA are incorrect, although the qualitative conclusion remains unchanged; IA is not to be understood as the first term in a standard series expansion. (2) The greater validity of IA for doubles than for the triples, which when integrated give doubles, is related to the existence of a sum rule, only valid for doubles. (3) The so-called "asymmetry" of a Compton profile is primarily to be understood as simply the shift of the peak position in the profile; symmetric and anti-symmetric deviations from a shifted Compton profile are very small, except for high Z inner shells where further p.A effects come into play. (4) Most relativistic effects, except at low energies, are to be understood in terms of simple kinematic modifications of non-relativistic IA, plus using a relativistic charge density for high Z inner shell states; these shift the peak and change its height.

Resonant X- Ray Diffraction Studies of Magnetism and Much More Materials Science

M. J. Cooper [1,2], C. A. Lucas[1,3], L. Bouchenoire[1], S. D. Brown[1], D. Mannix[1,4], P.Normile[1], D. F. Paul[1], P. Strange[5] and P. Thompson[1]

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[2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK.
[3]Department of Physics, Oliver Lodge Laboratory, University of Liverpool, Liverpool L69 7ZE, UK.
[4]Institut Néel, 25 Avenue des Martyrs, BP 166, 38042 Grenoble Cedex, France.
[5]School of Physical Sciences, University of Kent, Canterbury, Kent CT2 7NH, UK.

The relatively small x-ray interaction cross–section, for terms coupling the radiation to spin and orbital moments, is enhanced very significantly at resonance. This makes it possible for a number of magnetic spectroscopies to be used to probe the nature of the magnetism in bulk, thin film and multilayer materials. The XMaS beamline at ESRF has led the development of low

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temperature (1 Kelvin), high field (4 Tesla) environments, compatible with diffraction geometries and suitable for resonant diffraction studies, plus polarisation conditioning and analysis tools and, recently, electric field capability for the study of multiferroic materials. The useable energy range now extends down to ~2.2 keV which allows 4d and 5f magnetism to be studied as well as 3d ordering phenomena in the manganites, cobaltates and vanadates. We will review recent resonant scattering studies and also present illustrative examples of other wide-ranging research on the XMaS beamline.

Condensed Noble Gases for Direct Dark Matter Search

M. I. Lopes

LIP-Coimbra and Department of Physics, University of Coimbra, 3004-516 Coimbra, Portugal

The physics of noble gases permits a large array of detector technologies. Recent developments of detectors based on noble gases are enabling advances in particle physics and cosmological issues, one of them being the direct dark matter search. The evidence of the existence of a non-baryonic dark matter component of the Universe has been strengthened in recent years. This matter can be composed by heavy non-relativistic particles commonly referred to as WIMPs (Weakly Interacting Massive Particles). The direct method of detecting such particles is to look for the energy deposited when a WIMP scatters off a nucleus of a target/detector material. In these rare events, the nuclear recoil energies are expected to range from a few keV to a few tens of keV. The main challenge for these experiments is to discriminate between these rare events and the much higher rate background due to natural radioactivity. Among the most competitive experiments are those using detectors based on condensed noble gases.

The properties of condensed noble gases that make them so suitable for WIMP detection are summarized. Recent progress in the detection techniques based on those materials are reviewed and the current status of the experiments running or developing this type of detectors are presented. The most important recent advances are highlighted and pointers to the future are given.

Laser- produced X- Ray Sources

Lawrence T. Hudson

National Institute of Standards and Technology, USA

A formidable array of advanced laser systems are emerging that produce extreme states of light and matter. By irradiating solid and gaseous targets with lasers of increasing energies and decreasing pulse durations, new physical regimes of radiation effects are being mapped out for the first time in the controlled laboratory setting. The primary goal, which is being accomplished or pursued using a variety of techniques, is the realization of novel sources of x-rays with unprecedented characteristics, the mechanisms of which are in many cases still being elucidated. Examples include the megajoule-class of laser-produced plasmas designed in

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pursuit of alternative-energy and security applications and the petawatt-class of lasers used for fast ignition and x-ray radiographic applications such as medical imaging and real-time imaging of plasma hydrodynamics. As these technologies mature, increased emphasis will need to be placed on advanced instrumentation and diagnostic metrology to characterize the spectra, time structure, and absolute brightness of x-rays emitted by these unconventional sources; such measurements provide the determination of plasma composition, density, and temperature as well as the conversion yields of laser light to x-rays. Such customized and absolutely calibrated measurement tools will serve as an enabling technology that can help in assessing overall system performance and progress, as well as the identification of the underlying interaction mechanisms of interest to basic and applied high-field and high-energy-density science.

Characteristic X- Ray Spectra : Developments in Understanding, Status and Future Opportunities

Jorge E. Fernandez[1] and Viviana Scot[1]

[1]*Laboratory of Montecuccolino-DIENCA, Alma Mater Studiorum University of Bologna, via dei Colli 16, 40136 Bologna, Italy*

It is well known that, due to Heisenberg's uncertainty principle, the energy levels in the atom are defined within an energy width (level width). Electronic transition involving two or more levels shows a natural width given by the sum of the widths of the participating levels. Accordingly, characteristic lines appear to follow Lorentzian-like distributions with the natural width being the FWHM.

Since a Lorentzian distribution has long tails on both sides, these tails may cross above neighbouring absorption edges giving rise to enhancement effects of a certain complexity.

In this article we describe systematically the self enhancement effects on XRF K-lines in pure element samples having atomic numbers Z=11-92. Secondly, we discuss the effect in the more complex case of L edges. Finally, we consider the case of multielement samples where K and L edges corresponding to different elements are overlapped. The study is performed by means of both deterministic and MC calculations.

The impact of this effect on the measurement of important atomic parameters like the fluorescence yield is discussed.

../Abstracts continued

Latest Developments and Opportunities for 3D Analysis of Biological Samples by Confocal µXRF

Roberto D. Perez[1 2 3], Hector J. Sanchez[1 2], Carlos A. Perez[4] and Marcelo Rubio[1 2 3]

[1]*FAMAF, Universidad Nacional de Córdoba, (5000) Ciudad Universitaria, Córdoba, Argentina*
[2]*CONICET, Rivadavia 1917, (1033) Buenos Aires, Argentina.*
[3]*CEPROCOR-Agencia Córdoba Ciencia S.E, (5164) Santa María de Punilla, Córdoba, Argentina.*
[4]*Laboratório Nacional de Luz Síncrotron—LNLS, POB 6192, 13084-971 Campinas, SP, Brazil*

The X-ray fluorescence analysis performed with primary radiation focused to micrometer dimensions is known as micro X-ray fluorescence (µXRF). It is characterized by a penetration depth higher than other microanalytical methods reaching hundreds of micrometers in biological samples. This penetrative characteristic of X-ray beams can be employed to advantage in 3D analysis. An innovative method to perform 3D analysis by µXRF is the confocal setup.

The confocal setup consists of X-ray lenses in the excitation as well as in the detection channel. In this configuration, a micro volume defined by the overlap of the foci of both X-ray lenses is analyzed. Scanning this micro volume through the sample can be performed in three dimensions.

At present, X-ray lenses used in the confocal µXRF experiments are mainly glass capillaries and polycapillaries. Glass capillaries are used in the excitation channel with sources of high photon flux like synchrotron radiation. Half polycapillaries or conical polycapillary concentrators are used almost exclusively in the detection channel. Spatial resolution of the confocal µXRF depends on the dimensions of the foci of both X-ray lenses. The dimensions of the probing volume reported in confocal µXRF experiments are of order of few tens of μm^3 .

In our confocal setup, we used a commercial glass monocapillary in the excitation channel and a monolithic half polycapillary in the detection channel. The polycapillary was home-made by means of drawing of multibundles of glass capillaries in a heating furnace. The experiment was carried out at the beamline D09B-XRF of the Synchrotron Light National Laboratory (Laboratório Nacional de Luz Síncrotron, LNLS) with a white beam.

A model for theoretical description of X-ray fluorescence intensity registered by confocal µXRF was introduced by Malzer and Kanngieber in 2005. These authors showed the scan of the X-ray fluorescence intensity is the spatial convolution of the sensitivity and the X-ray fluorescence emission rate to the detector. In a previous work we showed the convolution theorem can simplify the calibration and quantification process in confocal µXRF. In the present work, we applied these ideas to analyze by confocal µXRF samples of aquatic plants and a sample of tooth. We show that confocal µXRF can be successfully applied to help the study of the effects of water bioremediation on aquatic plants. We also show that confocal µXRF can be used to make topological studies of teeth.

../Abstracts continued

Major Scientific Developments at Synchrotrons and at the Australian Synchrotron, and Prospects for Future Directions

Robert Lamb

Australian Synchrotron, Clayton, VIC, Australia

Australia's newest and brightest major national research facility, the Australian Synchrotron, is open for business – and actively looking to attract research groups from around Australia and overseas.

Since officially opening our doors in July 2007, we have drawn hundreds of prospective users keen to use our unique capabilities to further their research objectives.

To many users, the synchrotron is simply a highly intense source of light ranging from infrared to hard x-rays. The unique properties of synchrotron light mean that experimental results are far superior in accuracy, clarity, specificity and timeliness to those obtained using conventional laboratory equipment.

Individual beamlines filter and direct selected wavelengths into customised experimental facilities, enabling an impressive array of non-destructive, high resolution, rapid, in-situ, chemical information from diverse sample types ranging from biological to industrial materials real-time imaging and analysis techniques. These can generate elemental, structural and and minerals.

The Australian Synchrotron is a world-class young facility with a rapidly growing reputation for producing high-quality results. By the end of 2009, we will be the largest scientific user facility in the southern hemisphere. As one of the newest facilities in the Asia Oceania region we are keen to show the world this fantastic facility which will underpin research in this region for years to come.

Synchrotron-based Techniques in Mineral Exploration

Joël Brugger[1,2], Frank Reith[2,3], Barbara Etschmann[1,3,4], Weihua Liu[1]

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[4] CSIRO Exploration and Mining, 3168 Clayton.

The World's appetite for metals (e.g., Au, Ag, Cu, Mo and U) is growing, but many of the World's greatest mineral deposits were discovered more than 100 years ago, and despite increasing spending on exploration, the rate of new discoveries is decreasing. This is due to the fact that outcropping deposits have been discovered.

Now exploration companies need to target deposits buried under many 10's to 100's of metres of barren rock and soil, leading to increasing costs while success rates decline. In this context, it becomes critical to understand the physics and chemistry leading to the formation of ore

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deposits in order to model the geological processes involved quantitatively. The aim is to integrate this information with traditional 'geo'-datasets (e.g., regional geology, geophysics, and geochemistry) to select attractive targets for drilling.

Synchrotron radiation is contributing to this endeavour in many ways, including (i) characterization of the biochemical controls on metal mobility in soils, in order to predict the geochemical footprint of a buried mineral deposit; (ii) support the modelling of ore transport and deposition, by providing molecular-level understanding of solvents and thermodynamic properties for the important metal complexes in brines, vapours, and supercritical fluids over the range of conditions relevant for the formation of mineral deposits (i.e., temperature 25-600°C; pressure 1 to Gpa; and fluid compositions varying from hypersaline (e.g., >50wt% NaCl) to volatile-rich (e.g., CO_2, CH_4, H_2S); (iii) track the fluids that travelled through rocks and predict their ore-forming potential by analysing hydrothermal minerals and remnants of those fluids trapped in these minerals (so-called 'fluid inclusions').

X-ray fluorescence and X-ray absorption spectroscopy are the two most common techniques used in support of mineral exploration. These samples pose great challenges to the techniques, in particular because of the (i) complexity of the heterogeneous samples, which often contain only low concentrations of some critical elements; (ii) beam sensitivity, especially for redox-sensitive elements in aqueous fluids or biological samples; (ii) extreme sample environments, e.g., in-situ study of fluids at high pressure and temperature.

Thus, critical improvements need to be made on a number of fronts in order to obtain: (i) more efficient detectors, able to map large areas in heterogeneous samples (e.g., 10^6-10^8 pixels per map), and also to collect a maximum number of photons to limit sample exposure and beam damage; (ii) integrate techniques (e.g., XRF, XAS, XRD) on single beamlines; (iii) advance the theory (e.g., quantitative XANES interpretation; XERT measurements), to gain maximum information from the hard-won datasets.

Reflections on Eighty years of progress in Electron-Atom Scattering

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The study of electron-atom collisions has been a major endeavour both experimentally and theoretically since the birth of quantum mechanics in the 1920's. It is quite remarkable that while major advances have been made in these studies, we are still carrying out investigations for the many of the same systems some eighty years later! This suggests that there are aspects of the quantum theory of scattering, particularly as it relates to particles with coulomb charges, that are still extremely challenging.

This talk will outline the development of our understanding of electron-atom collisions during those eighty years, using as our vehicle the non-relativistic Schrödinger equation. A discussion of some of the early theoretical work is appropriate if simply to illustrate the quality of the

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early contributions. The interplay of experiment with theory is emphasised as is the increasing realization that analytic methods and models are generally inadequate at lower energies and that progress could only be made with increasingly sophisticated numerical calculations. It is no coincidence that the most dramatic progress in computational methods has occurred since the late 1960's and closely parallels the rate of increase in speed and memory of computers since that period. The last part of the talk will discuss progress in the aspects of the three-body coulomb problem that are relevant to electron-atom ionisation and include some suggestions for future work.

Accurate Measurement and Physical Insight : The X-ray Extended Range Technique for Fundamental Atomic Physics, Condensed Matter Research and Biological Sciences

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Research in core physics or atomic and condensed matter science are increasingly relevant for diverse fields and are finding application in chemistry, engineering and biological sciences, linking to experimental research at synchrotrons, reactors and specialised facilities.

Over recent synchrotron experiments and publications we have developed methods for measuring the absorption coefficient far from the edge and in the XAFS (X-ray Absorption Fine Structure) region in neutral atoms, simple compounds and organometallics reaching accuracies of below 0.02%. This is 50 - 500 times more accurate than earlier methods, and 50 - 250 times more accurate than claimed uncertainties in theoretical computations for these systems. The data and methodology are useful for a wide range of applications, including major synchrotron and laboratory techniques relating to fine structure, near-edge analysis and standard crystallography. Experiments are sensitive to theoretical and computational issues, including correlation between convergence of electronic and atomic orbitals and wavefunctions.

Hence, particularly in relation to the popular techniques of XAFS and XANES (Xray Absorption Near-Edge Structure), this development calls for strong theoretical involvement but has great applications in solid-state structural determination, catalysis and enzyme environments, active centres of biomolecules and organometallics, phase changes and fluorescence investigations and others. We discuss key features of the X-ray Extended Range Technique (XERT) and illustrate applications.

Crystallography Without crystals

Peter Colman

Walter Eliza Hall Institute, Australia

A retrospective of the development of phasing methods deriving from Shannon's theorem.

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Recent and Future Developments in the Use of Radiation for the Study of Objects of Cultural Heritage Significance

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Improvements in the design of synchrotron radiation sources have made it possible to undertake experiments on objects of cultural heritage experience which had hitherto been impossible. These experimental techniques range from X-ray diffraction and fluorescence (both micro- and macro-diffraction), XAFS and XANES (both micro-and macro-scattering), and infrared microscopy, and have been used in:

- the study of materials ranging from Australian Aboriginal bark paintings and other artefacts,
- the iron-gall inks on parchment in situ studies of corrosion processes

This paper will discuss investigations of important artefacts of cultural heritage significance, largely held by Australian national collecting agencies, using many different analytical techniques. All the investigations involve the use of radiation, either particulate, electromagnetic, or both. Early investigations used laboratory based equipment. Some of these include:

- investigation of the Carley Float from the HMAS Sydney (scanning electron microscopy/energy dispersive X-ray analysis)
- a study of the composition of eighty two Victoria Crosses held by the Australian War Memorial and the New Zealand Army Museum (X-ray fluorescence analysis)
- an investigation of the armour of the bushranger, Joe Byrnes, one of the notorious Kelly gang (gamma-induced X-ray fluorescence analysis, transmission electron microscopy)
- a study of inclusions in the semi-precious mineral, rhodonite (Infrared Raman microscopy)

A discussion will also be given of the use of particle beams (neutrons and protons) to study:

- the age of ceramics and glazes found in archaeological excavations (neutrons)
- the provenance of Aboriginal artefacts (PIXE), and the
- the debasement of Visigoth coinage (PIXE).

Characterization of a Prototype Linear Array Neutron Detector

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Neutron scattering experiments provide important information about crystalline structure, stresses and strains in materials, order and disorder at the atomic scale, effects of magnetism on materials, and so forth. The Spallation Neutron Source (SNS), located at Oak Ridge, TN, will offer researchers from around the world unprecedented neutron fluxes in a variety of beam lines, when it comes fully on-line in the near future. Our group at Kansas State University is

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building a thousand channel linear array neutron detector for use on the Vulcan beam line at SNS. The device will be composed of 64-channel modules that are made of perforated silicon, whose perforations are filled with ^{6}LiF and whose top surface also is covered by a thin layer of ^{6}LiF. This design allows thermal neutron detection efficiencies of over 20% to be achieved. Each 120-μm wide channel is read out by specially designed electronics. A 32-channel prototype module has been constructed and is now being tested at the SNS. The design, construction, and characterization of this prototype device will be discussed. The completed detector array will be one centimetre wide by four centimetres long and will be installed at SNS for neutron scattering studies.

Biomedical Applications of X-ray Absorption and Vibrational Spectroscopic Microscopy in Obtaining Structural Information from Complex Systems

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Hard X-ray microprobe techniques: synchrotron-induced X-ray emission (SRIXE) for elemental mapping at a sub-micron level; micro-XANES (X-ray absorption nearedge structure) for chemical information; and differential phase contrast (for mapping of morphology); are providing unprecedented information on biotransformations of drugs, toxins and carcinogens, as well as normal biological processes and disease conditions at the molecular and cellular levels. These techniques can be complemented by vibrational spectroscopic mapping/imaging and/or fluorescence images of the same cells, which provide information on changes in biochemical distribution, concentrations and secondary and tertiary structure of biomolecules in cells under disease conditions or during the treatment of diseases. When combined, these microprobe techniques can provide information that can lead to improved drug design to maximise efficacy and reduce side-effects, and to provide early warnings of potential hazards of certain treatments.

Biomedical applications of microprobe and bulk X-ray absorption techniques, and vibrational spectroscopy techniques will be discussed with respect to:

- the biotransformations and biodistributions of anti-diabetic Cr dietary supplements and the potential risks of taking such supplements;
- the biotransformations and biodistributions of anti-diabetic V drugs; and
- understanding the earliest stages of cardiovascular disease and damage and possible methods for their prevention and treatment.

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Applications of condensed matter understanding to medical issues and disease progression: elemental analysis and structural integrity of tissue scaffolds

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Synovial joints articulate in a lubricating environment, the system providing for smooth articulation. The articular cartilage overlying the bone consists of a network of collagen fibres. This network is essential to cartilage integrity, suffering damage in degenerative disease of the articular cartilage such as osteoarthritis. In work conducted by us at several European synchrotron sites and elsewhere we have been applying a number of techniques to study of the cartilage-bone interface and of changes occurring in this with disease and other influencing factors. Other tissue types in which we have examined the effects of disease processes are the basement membrane of lens and breast tissue. The techniques applied include x-ray phase contrast imaging, X-ray fluorescence mapping and coherent small-angle X-ray scattering (cSAXS), yielding information on anatomical features, elemental make-up and the large scale organisation of collagen. The talk will present examples of the results obtained to-date.

Application of XAFS to Biologically-Relevant Metal-Based Chemistry

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Notwithstanding the considerable advances in computational methods, elucidation of the pathway of chemical reactions depends critically on the identification of intermediates. In many cases the lack of samples suitable for crystallographic analysis then requires that the structures be deduced using spectroscopic and computational methods. The paper focuses on the integration of spectroscopic, computational (density functional theory, DFT) and EXAFS (extended X-ray absorption fine structure) methods to allow assignment of the structures of reactive electrogenerated compounds.

A key focus of this work is the elucidation of the reduction chemistry of compounds with structures related to the active centre of the [FeFe] hydrogenase enzyme. Methods used for sample collection and validation are crucial to the acquisition of meaningful results and this together with the integration of the computational/XAFS results with those obtained using range of spectroscopic (IR, EPR and/or UV-Vis) and physical techniques will be discussed.