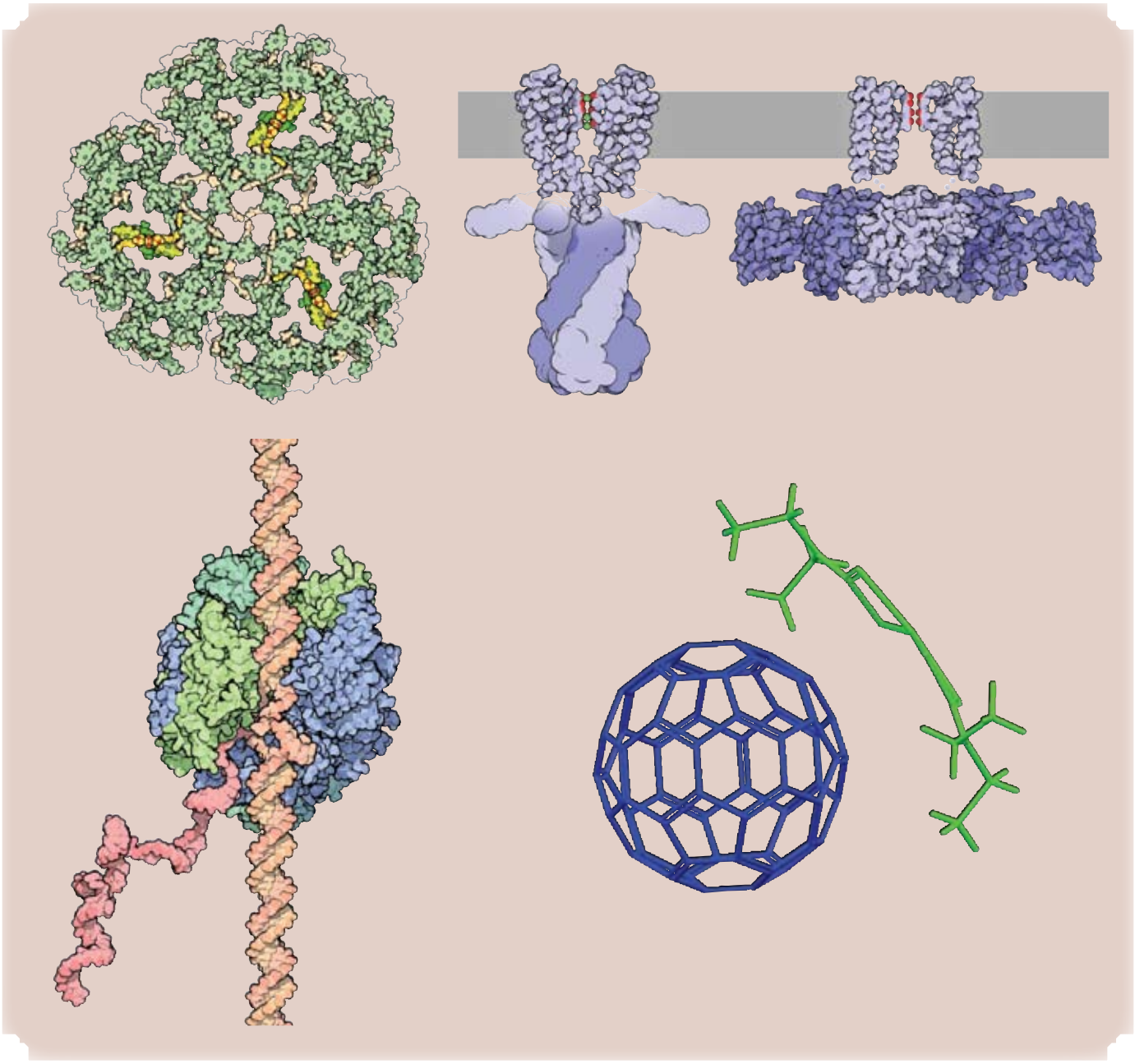
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

Number 2

Summer 2007



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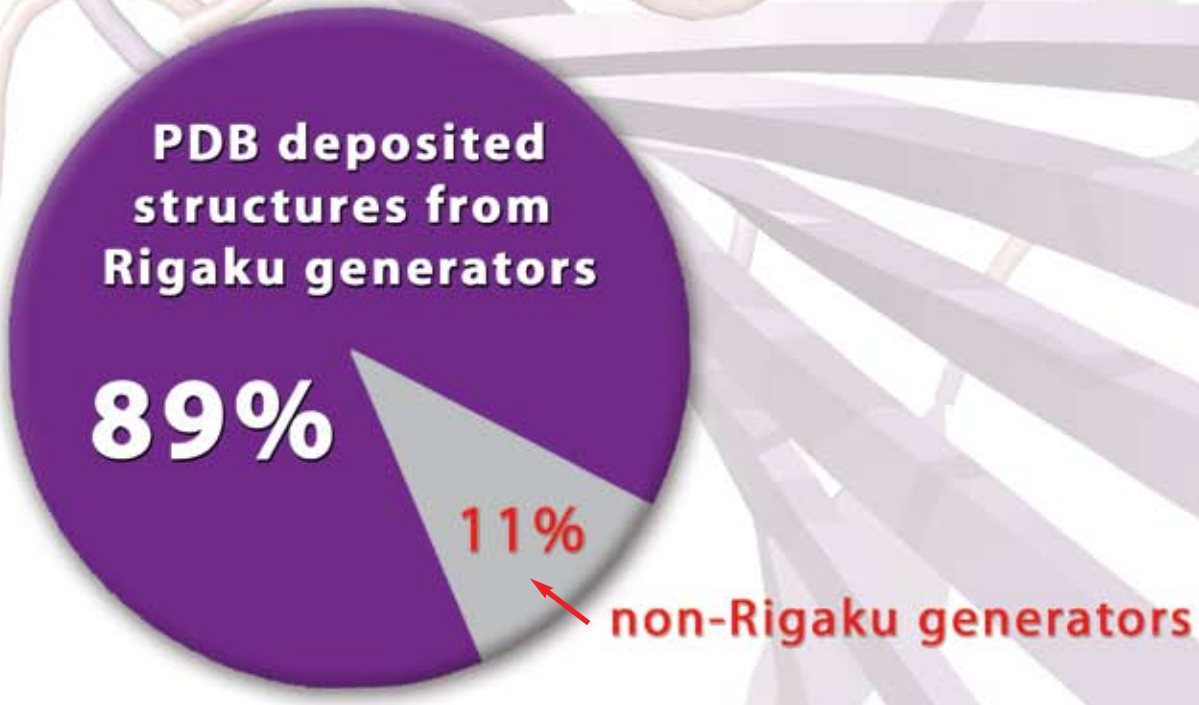

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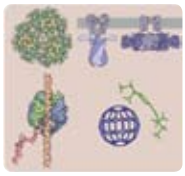

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President's Column

For those of us in academe, this is the end of the academic year, and so our thoughts turn to the summer conference schedule. I anticipate that our meeting in Salt Lake City will be a great success, not only because of the excellent program that you can find on the ACA web site, but also based on the hard numbers – 518 abstracts were received, most of which are available on the web. Since the last edition of *RefleXions*, there has been a modification to the program. As many of you are aware, F.A. Cotton passed away in February, the consequence of injuries received during an assault last fall. Clearly, Al had a major influence on the way that small molecule crystallography developed into the essential tool that it has become for all those involved in chemical research. The session "Important Science from Small Molecules" organized by Larry Falvello and Allen Oliver addresses and celebrates the kind of crystallography that was emphasized in the Cotton laboratory. For this reason, the session is being offered as a tribute to Al's contributions and will include a retrospective of his work presented by Larry.

Although most of the ACA awards are given on a three year rotation, the Margaret C. Etter Early Career Award is given annually. At the spring council meeting, we discussed the advisability of changing the nomination procedure for this award. In order to have additional input from the younger members of the ACA, and to encourage a greater breadth of nominations, the deadline has been moved to September 1 so that it will be after the annual meeting. Please discuss possible nominations with your colleagues during the meeting.

I encourage all of you to participate in the annual business meeting that will take place at the end of the scientific sessions on Wednesday, July 25. Along with the usual reports on such topics as the financial health of the organization, we would like to hear your opinion on the possible cost savings of providing abstracts in electronic form rather than printing and shipping full program and abstract books. Another topic of discussion will be the possibility or advisability of combining meetings with the Denver X-ray Conference. Clearly, we are all crystallographers, and many of us attend both meetings. I note that there have been increasing numbers of sessions on powder methods at the ACA meetings in recent years, and that will again be the case in Salt Lake City.

I would like to finish with comments on some broader concerns. At a recent meeting of the Council for Scientific Society Presidents, there was much concern about the state of science and math education. Despite the expressed desire to implement national standards and emphasize STEM areas that we have all seen in the press, the council identified a major flaw in this process – the lack of subject training in the backgrounds of many of our teachers. To those of you who have influence on curricular decisions in your institutions, please encourage such concepts as joint science/education programs, where the science or math is taught by the appropriate academic departments, not a watered down version only acceptable to the education faculty. Reading "Rising Above the Gathering Storm" published by the National Academy of Sciences will convince you that the time to act is now if we are not to become an economic backwater.

You will find below a guest editorial from the local chair of this year's meeting. This editorial addresses another scientific concern within the rubric of scientific responsibility – the concepts of energy conservation and global warming. In particular the appeal is "Make the 2007 ACA Conference Climate Neutral." The article will provide details of how you might contribute to this effort.

In closing, I encourage you all to continue to apply your scientific abilities to the endeavors that make the ACA such a vibrant organization, and to always be conscious of the potential to help address questions of societal and global inport.

Alan Pinkerton

Making the 2007 ACA Meeting Climate Neutral

Science is the search for an objective understanding of the way things are and work. The best scientists are intellectually ambitious, rigorous, and creative. They are independently minded and instinctively look for the weaknesses and alternative explanations in the work of others. Therefore, when scientists in a large and dynamic field reach a consensus their collective opinion should be taken very seriously. So it is with Global Climate Change, where strong scientific consensus states that human activity is on track to cause worldwide challenges that within a few tens of years are likely to be very serious and possibly catastrophic.

We therefore hope that members of the ACA will join our effort to make the 2007 annual meeting Climate Neutral. We cannot prevent all greenhouse gas emissions, but we can ensure that the net result of our activities decreases rather than increases the amount of CO_2 in the atmosphere. This goal can be achieved by offsetting the CO_2 released as a consequence of attendees and vendors flying to the meeting and using the conference center and hotels. There are two general approaches to achieving this goal, conservation and alternative technologies, both of which will be used.

Thoughts of conservation typically include fuel-efficient vehicles, telecommuting, public transportation, compact fluorescent light bulbs, and turning off lights, printers, and computers when not in use, all of which are important. We are going to take the alternative approach of supporting a tropical rainforest preservation/reforestation program. These programs allow local people to develop out of poverty through activities such as highly sustainable harvesting and ecotourism, thereby preventing the release of CO_2 through burning/clearing of forest for unsustainable harvesting of wood or for agriculture. This mechanism is effective in preventing CO_2 release and, as with most good ideas, there is more than one benefit. Destruction of rainforests causes about 25% of all CO_2 emissions. In 1950 tropical rainforests covered about 14% of the earth's land surface, today it is about 7%, and it is projected that at the current rate of loss they will have largely disappeared in 40 years. Rainforests have been called the lungs of the planet and may be home to more than 50% of the world's species. Their loss would be an epic calamity, and for these reasons we have pledged to offset CO_2 emissions associated with the meeting by rainforest preservation. At press time, the exact details of this purchase are still being negotiated, but will probably offset about 50% of the emissions associated with the meeting. Details will be announced at the meeting and reported in future issues of ACA *RefleXions*.

We have also established a wind energy campaign that will allow attendees and vendors to additionally offset the consequences of CO_2 emission, with total contributions for the ACA campaign updated and posted monthly (***windpower.utah.edu***). Most of our electricity is produced from burning coal, a process that causes more than 30% of the total CO_2 emissions in the USA. Furthermore, use of coal to produce electricity causes 40% of all mercury pollution in the USA and the EPA recently announced that one sixth of US women of childbearing age carry mercury above their level of concern for the fetus. In contrast, production of electricity from wind has very low environmental impact, it is highly cost effective, and the potential for its increased utilization is huge. According to the US Department of Energy we could produce 150% (yes, 150%!) of our electricity from wind, although the current amount is just 0.6%. In contrast, Denmark currently makes more than 20% of its electricity from wind and has recently announced plans to increase this to 50% by 2025. Our campaign is run through the University of Utah and, to the best of our knowledge, it is the most cost effective way for individuals to fund wind energy in the country. The donations fund construction of new wind turbines that serve the Western US grid and, because of the 1978 energy act, they will necessarily displace the use of fossil fuels, especially coal. The program costs just $3 per mwh and represents a 5% increment on the standard residential electricity rate. Moreover, donations to this campaign are tax deductible. The impact of an average domestic US flight would be offset by a donation of $5 ($3 if accounting for just your own coach class seat but not considering empty or first class seats) and the total impact of an average attendee at the meeting (conference center and hotel) would be offset by an additional $2. This campaign is also an effective mechanism to mitigate other sources of emission. For example, electricity used by an average university worker ($30/year), an average US household's electricity ($30/year), an average US family's total direct fossil fuel use, excluding air travel, ($90/year).

It is lamentable that the serious warnings about climate change from a remarkable scientific consensus is not being taken more seriously by policy makers. To some extent this is understandable because politicians are obliged to consider input from innumerable sources, including major industries that help drive economic processes that often have a huge resistance to change. As scientists we share a responsibility to raise awareness of the true consensus in our community, accept personal responsibility, and show leadership by taking meaningful action to address the issues directly. We hope that you will join our efforts to make the 2007 ACA meeting Climate Neutral by donating to the ACA campaign on the ***windpower.utah.edu*** web site.

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Thomas C. Terwilliger
Liang Tong
Jill Trewhella

NOTE:

We are advocating a specific campaign because we believe that it is the most cost effective option for individuals to offset their CO_2 emissions and because it allows a campaign approach in which ACA members and friends can work collectively to achieve a significant goal. It is important to note, however, that there are many other programs that one might choose to support, including those listed here.

Carbon Offsets:

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www.carbonfund.org
www.nativeenergy.com
www.paxnatura.org
windpower.utah.edu

Other Links:

www.climatecrisis.net
www.carbontradewatch.org
www.ucsusa.org

Creationism Going Global

The February 16, 2007 issue of *Science* included an article by Martin Enserink titled "In Europe's Mailbag: A Glossy Attack on Evolution." The consensus among European scientists that received unsolicited free copies of the 768 page, lavishly produced, *Atlas of Creation* was that it is the most gorgeous-looking attack on evolution seen in a long time.

The book was written by a Turkish author, Harun Yahya, who denounces Darwinism as the source of many evils. The book was sent to hundreds if not thousands of researchers in at least four countries in western Europe. A source of amusement to some, the book has troubled and outraged others, especially in France, where a French translation showed up at hundreds of high schools and libraries.

The following update was sent out by the National Center for Science Education (***www.ncseweb.org***), the organization that tracks and archives information on the creation controversy.

A special report in the April 19, 2007, edition of *The Economist* --datelined "Istanbul, Moscow, and Rome" -- discusses the continued global spread of creationism. The incidents discussed are the dissemination of a book preaching Islamic creationism in France, the controversy over the display of hominid fossils in Kenya, the unsuccessful lawsuit over teaching evolution in Russia, and, at length, the current discussion within the Catholic Church. Creationism, the article suggests, is likely to continue to spread, especially in the developing world where fundamentalist versions of Christianity and Islam are expanding. The report notes, "As these examples from around the world show, the debate over creation, evolution and religion is rapidly going global. Until recently, all the hottest public arguments had taken place in the United States, where school boards in many districts and states tried to restrict the teaching of Darwin's idea that life in its myriad forms evolved through a natural process of adaptation to changing conditions." *Kitzmiller v. Dover* is cited as delivering "a body-blow" to "Darwin-bashers": "the verdict made it much harder for school boards in other parts of America to mandate curbs on the teaching of evolution, as many have tried to do -- to the horror of most professional scientists."

For the full story visit: ***www.economist.com/world/displaystory.cfm?story_id=9036706***

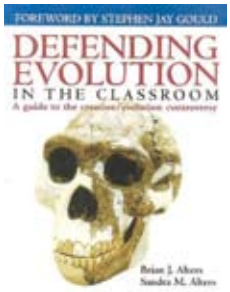
Meanwhile – A new attack is launched back home in the USA: On May 28th, the young-Earth creationist ministry, Answers in Genesis, opened a new creationism museum in Petersburg, Kentucky, just south of Cincinnati, Ohio. The Creation Museum will present a "walk through history." Designed by a former Universal Studios exhibit director, this state-of-the-art 60,000 square foot museum will bring the pages of the Bible to life. It will provide a fully engaging, sensory experience for guests including murals and realistic scenery, computer-generated visual effects, over fifty exotic animals, life-sized people and dinosaur animatronics, and a special-effects theater complete with misty sea breezes and rumbling seats.

The National Center for Science Education is asking concerned scientists in Ohio, Indiana, and Kentucky to visit ***sciohost.org/states*** to see ways in which they might become involved locally in efforts to protect the integrity of science education.

For more information: go to ***www.aaas.org/evolution***. To request a free DVD copy of the AAAS video on evolution, or the Project 2061 Abbreviated Guide to Teaching Evolution, e-mail Angela Bradley at ***abradley@aaas.org*** .

Books:

Defending Evolution: A Guide to the Evolution/Creation Controversy Brian J. Alters and Sandra M. Alters (2001), ISBN 10: 0763711187 (paperback), Jones and Bartlett Publishers, Sudbury, MA.



Defending Evolution is a novel handbook that explains why so many secondary and college students reject evolution and are antagonistic toward its teaching. *Defending Evolution* helps science instructors better understand their students' Creationist beliefs (including those of Intelligent Design advocates) and the bearing those beliefs have on learning evolution. The book provides instructors with a variety of concise, pragmatic suggestions to help lessen students' anxieties about evolution and to facilitate teaching.

From the foreward by Stephen Jay Gould: I particularly appreciate the authors' subtle understanding of the range of Creationist beliefs and motivations – thus avoiding a harmful caricature of all creationists as Bible-thumping literalists. The complexity of the subject can best be captured in two statements, emphasized throughout the book: 1. Most emphatically, creationism vs. evolution cannot be equated with religion vs. science. 2. Creationism spans an enormous range of beliefs and motivations. To be effective, teachers must vary their approaches to meet this enormous variety of concerns, tactics, and motives among creationist students and community members.

The book has chapters on why students reject evolution for both religious and non religious reasons and several chapters on questions and answers that provide a guide to 'defending' evolution in science and general education as well in religious issues.

Teaching Biological Evolution in Higher Education: Methodological, Religious, and Nonreligious Issues, Brian J. Alters (2005) ISBN 10: 0763728896 (paperback) Jones and Bartlett Publishers, Sudbury, MA.

An important new book by the author of the bestselling text *Defending Evolution: A Guide to the Creation/Evolution Controversy,* Teaching Biological Evolution in Higher Education examines the controversial issues surrounding this central concept of life science; explores students' common scientific misconceptions; describes approaches for teaching topics and principles of evolution, and offers strategies for handling the various problems some students have with the idea of evolution due to religious influences. This book is an indispensable resource for all instructors who teach aspects of biological evolution in their college courses. ***(from the publishers website)***

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News from Canada

Canadian Light Source News (from the CLS E-News, ***www.lightsource.ca/*** Recently $25.8 million was awarded from the Canadian Foundation for Innovation for three projects to be built at the CLS. The projects are led by teams from the University of Guelph, the University of Saskatchewan, and the University of British Columbia. Construction and operation will be done in collaboration with CLS scientists. "These investments represent a tremendous boost to Canada's research capacity," said CLS Executive Director Bill Thomlinson. "The support from CFI is helping us build critical infrastructure which positions the CLS as a global leader in synchrotron science." The three projects together comprise five new beamlines. Construction is expected to begin in early 2008, with some of the new facilities operational as early as 2011. The press release may be found at: ***www.lightsource.ca/media/media_release_20061127.php.***

The draft report from the Mid-Term Review of the CLS NSERC Major Resources Support Grant was presented at the Scientific Advisory Committee meeting, held November 13-14, 2006. The report is very positive on the progress and successes of the CLS in operations, science, and infrastructure development. Specific recommendations are currently being reviewed by CLS management for action.

The first publication resulting from experiments performed at the Canadian Macromolecular Crystallography Facility beamline was recently published in the *Journal of Biological Chemistry.* The paper is titled "Calcium Stiffens Archaeal Rad51 Recombinase from Methanococcus voltae for Homologous Recombination" (Xinguo Qian, Yujiong He, Xinfeng Ma, Yu Luo, and Pawel Grochulski) and is available online at: ***www.jbc.org/cgi/reprint/281/51/39380.***

Message from Bill Thomlinson: 2006 was an extremely eventful and productive year for the CLS. The announcement of $25.8 million in funding from the Canada Foundation for Innovation for three Phase III facilities, very positive results from our granting council mid-term review, and the first publications by users resulting from data obtained at the CLS will undoubtedly be the most recalled memories of the past year.

All of our Phase I beamlines are now running and producing original science and hosting outside users. In addition, first light in some of the Phase II facilities is anticipated by this fall.

The machine also continues to surpass original performance goals. The first tests of top-up mode were successful and we are looking forward to operations for users in top-up mode later in 2007. Regular operations at 250 mA, along with improvements in single bunch, multi bunch, and top-up modes will provide enhanced opportunities for our users on all of our Phase I beamlines.

Ernst Bergmann, User's Advisory Committee Chair-elect reports: The UAC has been busy with preparation of the 2007 Annual general Meeting (see below). Another issue of importance for users is the priority for the future machine capabilities of the CLS. Discussions on this issue are continuing. Among the options for future development are increased brightness, top-up mode, and 500 mA operations. The UAC is also concerned about the availability of sufficient resources for beamline development, especially engineering and control systems. With the development of phase I beamlines still ongoing, phase II beamlines in various stages of development and procurement and phase III beamlines funded, the UAC is encouraging the CLS to address possible shortfalls.

Jeff Cutler reports: With Phase I beamlines coming into full operation, the industrial science/business development group is becoming increasingly active. Within the last few months, the CLS has signed eight new contracts on projects ranging from macromolecular crystallography to air particulate emissions from smelters. A number of these are new customers, and a significant portion are repeat clients who see having access to a synchrotron a part of their core business. CVRD INCO Ltd., for example, one of the world's premier mining and metals companies and the world's second largest producer of nickel, has seen the synchrotron as so potentially important to its operations that they are considering investing in a dedicated CLS scientist to work on their projects.

In the next few months the CLS will be launching an industrial science advisory committee composed of both scientists and business representatives to help identify strategic directions for our group. We look forward to building capacity in our business development activities and industrial science program.

The industrial science group is involved in a number of different events taking place over the next several months, such as the Canadian Society for Chemistry conference in Winnipeg and the Synchrotron Radiation Instrumentation meeting in Baton Rouge, the key event in the North American synchrotron design community. Also noteworthy is a workshop to be held at the CLS Users' meeting on industrial applications of synchrotron light which will include leaders in commercial synchrotron applications. Simon Bare, from UOP LLC (a Honeywell Company) and Stewart McIntyre, former Director of Surface Science Western, are the keynote speakers. For more information go to: ***www.lightsource.ca/uac/meeting2007/workshop_indapp.php***

As a result of a Call for Proposals for beamtime in the July to December 2007 period the CLS received 65 proposals, plus 21 renewals. These are currently in review. The Peer Review Committee (PRC) will meet in mid-May and applicants will be notified of the results thereafter. Current members of the PRC include Chair Adam Hitchcock (McMaster) Bruce Bunker (Notre Dame), Jeffrey Cutler (CLSI), Karen Kavanagh (Simon Fraser), Shea Miller (Agriculture and Agri-Food Canada), John Tse (Saskatchewan), and Tony Van Buren (Lawrence Berkeley). The Chair serves a three-year term and the Committee members each serve a two-year term.

The Canadian Institute for Synchrotron Radiation (CISR) invites interested parties to participate in an online survey regarding synchrotron usage, both at the CLS and other facilities

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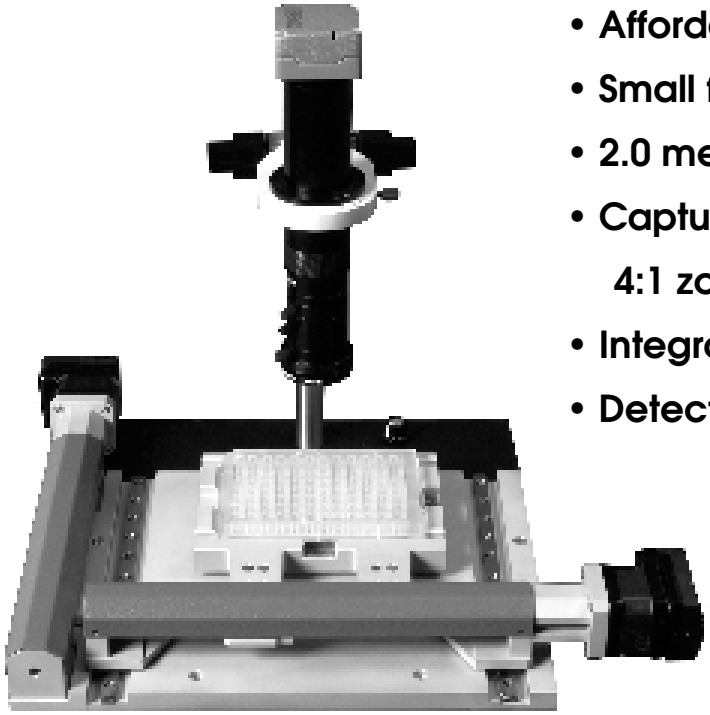

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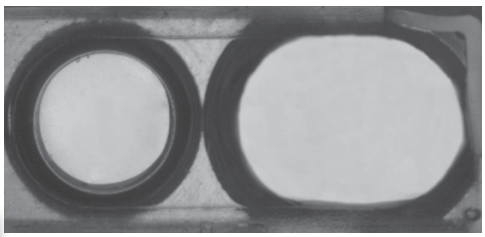

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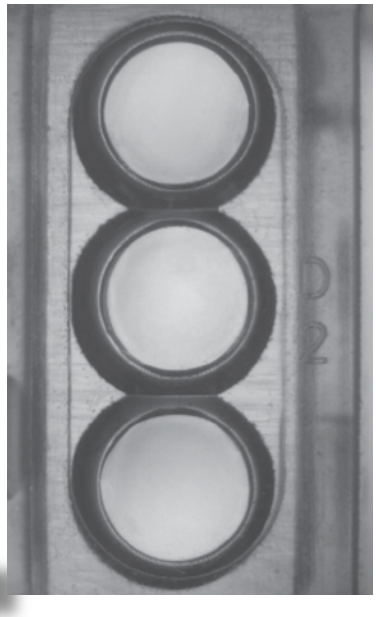

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outside Canada. Results from this survey will be discussed at the CISR annual meeting. The survey can be found at ***www.cisr.ca/survey/survey.html*** The User Name is "cisr" and the Password is "radiation".

Canadian Light Source Annual Users' Meeting and Associated Workshops

The Canadian Light Source Annual Users' Meeting and Associated Workshops was held at the University of Saskatchewan June16-17, 2007 in conjunction with the 62nd Annual Congress of the Canadian Association of Physicists June 17-20, 2007. Joint sessions were held on June 17th.

The AUM opened on Saturday, June 16th with a facility overview followed by the Keynote Speakers: ***Janos Kirz*** (Advanced Light Source), ***Dean Chapman*** (University of Saskatchewan), ***Serge Desgreniers*** (Université d'Ottawa), ***Andrew MacMillan*** (University of Alberta), and ***Kenneth Kemner*** (Argonne National Laboratory). There was also a special presentation by ***Christine Fitzgerald***, Executive Vice-President, Canadian Institutes of Health Research titled *The CLS - View from the CIHR*. The day ended with presentations on the latest results from the CLS and the Young Scientist presentations.

Joint workshops on June 17th included *Recent Advances in Condensed Matter Physics with Synchrotron Radiation, Recent Progress in Studying Biomaterials with Synchrotron Radiation, Illuminating to New Depths: Our Understanding of Surface Phenomena, Industrial Applications of Synchrotron Radiation, and Soft X-ray Spectromicroscopy for Biological Research.*

The Herzberg Public Lecture on the evening of June 17th featured Nobel Laureate Carl Wieman, co-discoverer of the Bose-Einstein condensate. This event was co-sponsored by the Canadian Association of Physicists.

The Canadian Institute for Synchrotron Radiation again offered a prize for the best synchrotron related poster presented by a graduate student or post-doctoral fellow. The prize is $1000 to support travel by the winner to attend and present their work at a related conference of their choice during the coming year.

Other activities during the AUM included tours of the CLS, a wine and cheese poster session, and a banquet Saturday evening featuring ***Herman Winick*** (Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, and Stanford University) speaking on "SESAME and the Impact of Synchrotron Radiation Research on Science and Society in Developing Countries".

For more information about the meeting and associated events see ***www.lightsource.ca/uac/meeting2007.***

Canadian Chemistry Conference and Exibition

The Canadian Society for Chemistry's 90th Canadian Chemistry Conference and Exhibition was held in Winnipeg May 26-30, 2007. Detailed information on the conference program is available at ***www.csc2007.ca/.***

International Meeting for Medical Applications of Synchrotron Radiation (MASR)

The International Meeting for Medical Applications of Synchrotron Radiation (MASR) will be held August 26-30 in Saskatoon. Confirmed speakers include ***Jacques Balosso*** (INSERM, France), ***Fulvia Arfelli*** (INFN, Italy), ***Alberto Bravin*** (ESRF, France), ***Diego Dreossi*** (INFN, Italy), ***Francois Esteve*** (INSERM, France), ***Ralf Menk*** (Elettra, Italy), ***Elisabeth Schültke*** (CLS, Canada), and ***Naoto Yagi*** (Spring 8, Japan). Abstract covering all techniques used to enhance better understanding, diagnosis and therapy of human or veterinary disease are invited. Topics include technical basics, X-ray imaging, SAXS, IR microspectroscopy, pathology, oncology, radiation biology, and radiology. To register see ***www.lightsource.ca/masr2007.***

Member News ***Endel Aruja*** reports that at 95 it is time for him to back out, with thanks to the crystallographic community.

Lee Groat

Notes from the AIP (Assembly of Scientific Society Officers and Governing Board) 28 March 2007

Each year in conjunction with the spring Governing Board meeting the AIP sponsors an exploration of public policy issues called the Assembly of Scientific Society Officers. This year provided an unusually lively program of four mini-symposia on physics in China, education in the US, diversity, and science funding.

This was the last Governing Board meeting for the retiring AIP CEO, Marc Brodsky. Testimonials at a dinner in his honor left no doubt that his mark on the AIP was extraordinarily positive. Several friends who were associated with the AIP in the distant past have written to me surprised that I was interested in an organization with so parochial a focus and suffering such internecine struggles. The answer is that Marc has transformed the AIP into both a strong financial organization and a vibrant public policy agent.

A particularly timely mini-symposium on diversity minorities noted that black physicists and geoscientists earn only 0.8% and 0.6% of the PhDs awarded annually in the US, despite the fact that black Americans as a whole earn more doctorates in all fields than do Asian Americans. Recognizing this, the AIP has provided for Member-at-Large representation on the Governing Board for Quinton Williams. Quinton is currently president of the National Society for Black Physicists and he has created an advisory committee to advise the AIP on underrepresented minorities. Several candidates have offered to represent the ACA on this new committee. The council is making a selection.

Two speakers at the convocation were AIP Congressional Fellows. They work on the staff of a member of Congress, and are crucial to the evaluation of science-related legislation. They provided very helpful insights into how science policy is decided and implemented. Other speakers expressed lavish praise for the fellowship programs. An important message to all ACA members is that fellowship appointments arise regularly, the experience is nearly always very positive, and the function of fellows is indispensable.

The AIP has participated in a very important data gathering study on attitudes toward the teaching of science and religion by two different polling organizations. Results were described in another mini symposium. 1000 likely voters were interviewed about their political and religious views, and their opinions of science. Nearly 60% of respondents attend some church regularly. A similar, but distinct, percentage was reluctant to breach the wall separating church and state. This overlapping population is where the battles will play out. Not surprisingly, much depends on how questions are asked. Swing voters are very likely to favor critical thinking, preparation for college and competitiveness in job searches, and drawing conclusions from evidence if questions are asked appropriately. The issue of fairness in contributing to critical thinking is also important, and may provide the wedge that allows creation science and intelligent design to win skirmishes every now and then. These data imply two conclusions for coming battles over the teaching of evolution and how science is done in general. First, the status quo is "our friend". Critical thinking is still favored by a majority. Second, a "SWAT team" is a more appropriate tool than a "standing army" in marshaling public policy efforts.

Finally, despite attempts of administration appointees to reassure the audience of scientific officers, the dominant message was shockingly contradictory. Overall, the mindset pervasive in the current administration that the US will remain the leading scientific power in the world is not only delusional but contradicted by statistics compiled over the past dozen years or more. A lively discussion among guests followed the presentation on the "No Child Left Behind" program. Statistics provided were no more recent than 2002 and were broadly questioned. A frequent skepticism voiced was that "Teaching to the Test" was counterproductive. Three speakers addressed the sea change occasioned by the 2004 congressional election. Long-time observers made it clear that the previous Congress was almost pathologically dysfunctional, and that the firewall erected by the Executive branch against oversight by Congress was explicitly called "appalling". Several speakers expressed hope that the new Congress will cauterize some of the wounds.

Charlie Carter

The ACA Patterson Award, established in 1980, is given every three years to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information. Previous winners of the A.L. Patterson Award are: 2005: ***Alwyn Jones***; 2002: ***Douglas Dorset***; 1999: ***Gerard Bricogne***; 1996: ***Christer E. Nordman***; 1993: ***George Sheldrick;*** 1990: ***Michael M. Woolfson***; 1987: ***David and Lieselotte Templeton***; 1984: ***Jerome Karle and Herbert Hauptman;*** 1981: ***Wayne A. Hendrickson***. The next Patterson Award will be made in 2008 (see the following article).

2008 ACA Patterson Award to Bi Cheng Wang

Bi Cheng (B.C.) Wang has been selected as the 2008 recipient of the ACA Patterson Award: "For significant contribution to the methodology of structure determination from single isomorphous replacement or single-wavelength anomalous scattering data and for its impact on structural biology."

Members of the selection committee were: ***Frank Fronczek, Paul Langan, George Sheldrick, and Victor Young.***

In the early 1980s, macromolecular structure determination was a tedious and time-consuming process. In addition to protein supply, x-ray intensity, single point detectors, and computing resources, a major bottleneck in the process was the preparation of the heavy atom derivatives required for phasing. This is because two or more isomorphous heavy atom derivatives were required for the multiple isomorphous replacement (MlR) method to work. lt was during this time that B.C. was faced with the problem of a protein (Bence Jones protein Pav) that formed only a single platinum derivative. Since the MIR technique could not be used, B.C. developed what was to become the first practical method for macromolecular structure determination from SIR or single wavelength anomalous scattering (SAS) data, a process he called noise filtering (also referred to as solvent flattening), that resurrected the technique of density modification. Working at the VA Medical Center in Pittsburgh, B.C. produced a suite of easy-to-use programs, including an innovative algorithm for automatic detection and generation of protein- solvent boundaries, called the lSIR/ISAS program package, which he freely provided to the community (including source code!).

It is interesting to note that in his seminal 1985 (*Methods Enzymol,* **115**, 90-112) paper on solvent flattening, B.C. showed through simulation that a structure of a 113-residue protein could be determined using only the sulfur anomalous scattering signal from a single disulfide, provided that the data were measured accurately enough. Now, 20 years later, structure determination using the sulfur anomalous scattering signal has gained considerable success, and SAS structure determination has supplanted both MIR and MAD as the most common method of *de novo* structure determination.

Throughout his long career B.C. has also contributed to crystallographic education as Director of the ACA Summer School, to synchrotron data collection as Director of SER-CAT at APS, and technological and methodological advances in the field as Director of the Southeast Collaboratory for Structural Genomics.

John Rose

2007 Gairdner International Award

HHMI investigator ***Thomas A. Steitz*** (Yale) is among five scientists who have been honored with the prestigious 2007 Gairdner International Award in recognition of their contributions to medical science.

Presented to medical scientists worldwide whose work is expected to significantly improve the quality of life, the Gairdner Award is one of the most esteemed awards in medical research. In 2007 the Gairdner Foundation honored Steitz and ***Harry F. Noller*** of the University of California, Santa Cruz for pioneering work that led to the identification of the detailed structure and function of the ribosome, the subcellular structure in which proteins are synthesized. Noller and Steitz established that RNA-catalyzed reactions are critical, and their work explains how many antibiotics work and how new ones can be developed.

2007 Cosmos Club Foundation Young Scholars Award:

Daniel de Lill has been named a Cosmos Club Young Scholar for his work in high -pressure crystallography and luminescence of metal-organic framework materials. Dan started at The George Washington University in 2003 after a year of graduate work at the University of Arizona. He received an M.Phil. degree in chemistry in May 2006, and has just completed his 4th year of graduate work at GWU, with an anticipated graduation date of May 2008. His research focuses on the synthesis and characterization of novel metal-organic framework materials of primarily the lanthanide elements. He also studies the properties of these materials in search of potential applications, with a focus on their luminescent behavior.

The 2007 Dorothy Crowfoot Hodgkin Award

The Dorothy Crowfoot Hodgkin Award, sponsored by Genentech, is granted in recognition of exceptional contributions in protein science which profoundly influence our understanding of biology. The 2007 award will be presented to ***Leemor Joshua-Tor*** (Cold Spring Harbor Laboratory) at the 7th European Symposium of The Protein Society for her outstanding achievements in protein structure-function relationships, particularly in nucleic acid-protein interactions. The citation states that she has consistently made insightful contributions in the areas of DNA and protein structural biology as well as seminal contributions to our understanding of how Papillomaviruses initiate DNA replication.

Elected to the National Academy of Sciences

DavidA.Agard, investigator, Howard Hughes Medical Institute, and professor, department of biochemistry and biophysics, University of California, San Francisco is one of the 72 newly elected members of the National Academy of Sciences. David's work focuses on using structural biophysics to understand the structural origins and unique abilities of proteins whose sole stability comes from kinetics and not thermodynamics, to survive extreme conditions. His work also focuses on the mechanism and structural dynamics of the hsp90 molecular chaperone and the mechanism by which the eukaryotic centrosome regulates microtubule assembly.

2007 Compton Award:

The Advanced Photon Source and the APS Users Organization have announced that the 2007 Arthur H. Compton Award was presented jointly to ***Andrzej Joachimiak*** (on the left) and ***Gerold Rosenbaum*** (on the right). This choice recognizes the worldwide stature of protein crystallography conducted at the Advanced Photon Source, the importance of this field of research, and the major roles played by Joachimiak and Rosenbaum. The award cites them for "pioneering advances and leadership in establishing the APS as a premier location worldwide for protein crystallography research."

Greg Petsko Elected President of ASBMB

Greg Petsko, currently the Gyula and Katica Tauber Markey Professor of Biochemistry and Chemistry at Brandeis University, has been elected president of the American Society for Biochemistry and Molecular Biology (ASBMB) . His current research focuses on a range of biochemical questions encompassing the structural basis of enzyme catalysis, the dynamic properties of proteins, the control of virulence gene transcription, and the biology of the quiescent state of eukaryotic cells. His term as president begins July 1, 2007.

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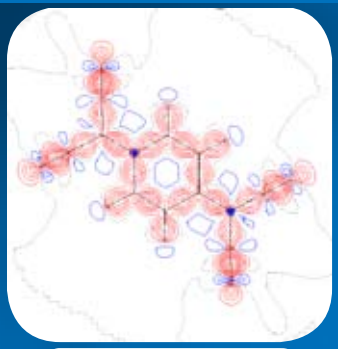

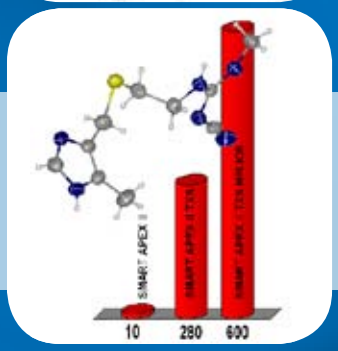

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Crystallography

Determining the Structures of Layered Materials by Neutron Reflection -Warren Award (2006)

Abstract: The evolution of neutron reflectometry and diffraction as a means for studying the nanometer- and Angstrom-scale structures of thin films and superlattices has spanned more than two decades. Several of the principal technical developments in theoretical analysis and experimental methodology that have enabled neutron reflectometry to become a significant contributor in a variety of scientific fields are discussed together with illustrative applications. The potential impact of future advances in neutron reflectometry techniques is also considered.

Introduction: It was recognized early on (see, for example, [1-4]) that neutron reflectivity (NR) measurements of layered materials can be a powerful means of probing the structure of a wide range of layered hard and soft condensed matter systems. The sensitivity of diffraction as a probe of laminar structures can be considerably enhanced if a given film of interest can be constrained to lie on a flat supporting surface or substrate. In the specular scattering condition, where the angles of incidence and reflection relative to the surface are equal, the wavevector transfer Q is normal to the surface and subsequent analysis of the reflectivity measured as a function of this angle yields the scattering length density (SLD) depth profile along the nominal surface perpendicular. This, in turn, can be related to the actual chemical composition profile. Using polarized neutrons, it is also possible to determine the vectorial magnetization depth profile in magnetic materials. Typical spatial resolutions can be of the order of a fraction of a nanometer. If the film is not homogeneous in a plane parallel to the surface, then off-specular scattering can reveal information about the nature of the in-plane density variations (in this brief survey, however, the emphasis is on specular scattering).

As is the case in other scattering methods, for example in powder diffraction, the underlying scattering theory describing either neutron or x-ray reflectivity is essentially equivalent. The differences primarily involve the details of the interaction between the radiation and the material, namely that x-rays scatter from the electrons and neutrons from the nuclei and any unpaired electrons of a given atom. So, as is well known, x-rays have an inherent sensitivity for discriminating between high- and low-Z elements in a given structure whereas neutrons have an advantage in distinguishing between hydrogen and deuterium.

What then distinguishes reflectometry, whether it be with x-rays or neutrons, as a special diffraction technique? Primarily it is the morphology of the sample as a whole being investigated, namely the flat, laminar form of a thin film or multilayer.

But in addition to the success in developing an experimentally optimized reflection geometry and a quantitatively accurate theoretical analysis of reflectivity data, the key to the emergence of neutron reflectometry as an important tool for structural investigations has proven to be the remarkable advances in various thin film deposition techniques. Notable among these are molecular beam epitaxy in ultra high vacuum, for hard condensed matter, and the Langmuir-Blodgett film transfer methods for soft matter systems. In general, given the ability to create layered structures with control on an atomic plane spacing length scale, innumerable possibilities arise for systematically studying various physical, chemical, and biological phenomena. Specific examples include: the behavior of electrons in neighboring layers, one of which is magnetic and the other super-, semi-, or ordinarily conducting or insulating; the lamellar ordering of diblock copolymers composed of two distinct species; the interaction of various macromolecular proteins with lipid bilayer membranes; and the diffusion of hydrogen into and through a host material film. The behavior of such tailored materials can be studied as a function of layer thicknesses or crystallographic orientation, which may be associated with strain caused by lattice spacing mismatch (as in the case of single crystalline layers or superlattices) or in contact with other media such as an aqueous fluid reservoir, with or without the application of an electrochemical potential.

Basic Principles: As already mentioned in the *Introduction*, measurements of the specular reflectivity as a function of Q, typically at grazing angles of incidence relative to the surface, can be analyzed to extract the SLD depth profile along the surface normal. The reflectivity, which is the ratio defined to be the reflected divided by incident intensity, is equal to the square of the modulus of the reflection amplitude which is related to the Fourier transform of the SLD (in the Born approximation where the assumption is made that the the scattering is elastic in nature and the wave function within the scattering medium is negligibly distorted from its plane wave form in vacuum). The Born approximation can be applied in the analysis of the diffraction from superlattices or multilayers where the Bragg-like reflections from a bilayer period occur at sufficiently large values of Q that the reflectivity is low enough that the underlying assumptions are valid. However, in a considerable fraction of cases, the Born approximation breaks down catastrophically at relatively low values of Q where the reflectivity can approach unity. Fortunately, there exists a quantitatively accurate, or so-called "dynamical" theory, based on the solution of the one-dimensional Schroedinger wave equation. This latter theory is routinely employed in the analysis of specular neutron reflectivity data. Within this formalism, reflectivity data collected up to wavevector transfers of the order of 0.5 inverse Angstroms, currently achievable in certain systems, can be analyzed to obtain SLD profiles with a spatial resolution of the order of a nanometer (for variations on that length scale; other features, such as the overall layer thickness of a relatively homogeneous film, can be obtained with Angstrom-scale resolution because of the inherent nature of the wave interference). Molecular dynamics simulations can be valuable in the subsequent step of relating the SLD to a chemical compositional profile. The minimum neutron reflectivities currently measurable are of the order of 1.0×10^{-7}. (For further discussion of of NR, see, for example, [5].)

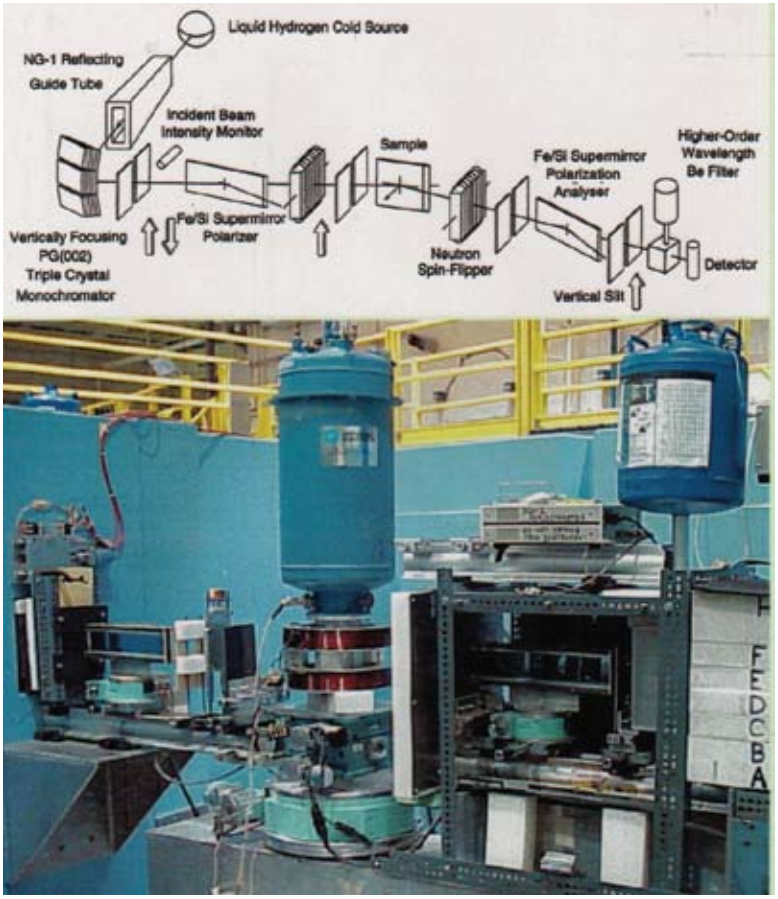


Figure 1. Polarized beam neutron reflectometer at NIST. The upper part of the Figure is a schematic showing essential optical components including pyrolytic graphite monochromator, beam defining apertures, supermirror polarizer and analyzer, and neutron spin rotators. The lower part of the Figure is a photograph of the actual instrument with the sample inside a cryostat and in between a pair of magnetic field coils.

The use of polarized neutron beams in reflectometry (PNR) allows the vectorial magnetization depth profile to be determined from spin-dependent specular measurements. The sensitivity to the direction of atomic magnetization in the sample follows from a set of scattering selection rules which depend upon the relative orientation of the magnetization, neutron polarization and wavevector transfer. The development of highly efficient multilayer or "super" mirror polarization devices have made the theoretically powerful PNR a practical realization. Used in conjunction with spin rotators of equally high or better efficiency, highly accurate, quantitative polarized neutron reflectivity data can be collected in routine fashion (e.g., see [6] for a detailed discussion).

Although the theoretical formalism described above is remarkably accurate in predicting the reflectivity curve to be expected for a model SLD profile, extracting a SLD profile from a measured reflectivity curve is another matter altogether. Since it is the reflectivity and not the reflection amplitude which is the experimentally measurable quantity, crucial phase information can be unavoidably lost. This, of course, is an age-old problem in crystallography as well. A complicating factor in reflectometry stems from the dynamical nature of the scattering which requires modified approaches in dealing with phase retrieval, as will be discussed in a separate section to follow. (For a review of phase-sensitive NR methods, see [7].)

The design of neutron reflectometers varies, depending, for instance, on whether the instrument is located on a continuous or pulsed source or whether the reflecting surface of the sample is vertical or horizontal relative to the earth. At pulsed sources polychromatic bursts of neutrons are incident on the sample and time of flight discriminates between different wavelengths, and, therefore, corresponding Q values arriving at the detector. At continuous sources, on the other hand, nearly monochromatic beams are incident upon the sample. The use of a horizontal sample geometry makes possible studies of liquid surfaces in contact with gaseous media. Figure 1 shows a schematic and photograph of one of the reflectometers at the NIST Center for Neutron Research, a continuous source with a liquid hydrogen moderator to enhance intensities at longer wavelengths (the nominal wavelength is 4.75 Angstroms). This instrument has the capability for using polarized beams, which are important not only for studying magnetic films but for performing phase determination in nonmagnetic films of interest via buried magnetic reference layers (see discussion in subsequent sections).

The Issue of Uniqueness: Figure 2 depicts a family of scattering length density profiles for a TiO/ Ti film system on a Si substrate in contact with an aqueous solution and at an applied electrochemical potential. The solid curves yield good fits to the measured neutron reflectivity data (inset) and were obtained by a model-free fitting scheme [8]. The differences among the curves are a measure of both the finite extent of the Q-range over which it was possible to collect reflectivity data, along with the statistical uncertainty associated with that data. However it is clear that there exists (at least) one other family of profiles (for clarity only one member is shown for clarity as a dashed curve) that possesses nearly, if not exactly, the same goodness of fit to the data (the corresponding reflectivity curve for this SLD profile is also plotted in the inset but is virtually indistinguishable from the others). Examples such as this abound and, as already mentioned above, are a manifestation of the loss of phase information when measuring the reflectivity as opposed to the complex reflection amplitude. It was discovered [10] about a decade ago that the reflection amplitude could be determined exactly, within the dynamical scattering theory based on the solution of the Schroedinger wave equation, by performing reflectivity measurements from a minimum of two composite thin film systems, both containing the common film of interest, the SLD profile of which is "unknown", but each including one or the other of two different "known" reference layers (or surrounding media). A simple linear set of equations can be solved which yields the real and imaginary parts of the reflection amplitude for the unknown part of the SLD profile in terms of the two measured composite reflectivity data sets and corresponding reference parameters independently, at any given value of Q. Once

the reflection amplitude has been so determined, the dynamical specular reflectivity, which can be described quantum mechanically as one-dimensional scattering, is exactly solvable by a first-principles inversion using the Gel'fand-Levitan-Marchenko integral equation[11]. That solution can, in fact, be proved to be unique (for reflectivity data obtained over the entire Q range). An example of a complete phase-sensitive measurement and subsequent inversion is given below in the section on scientific applications.

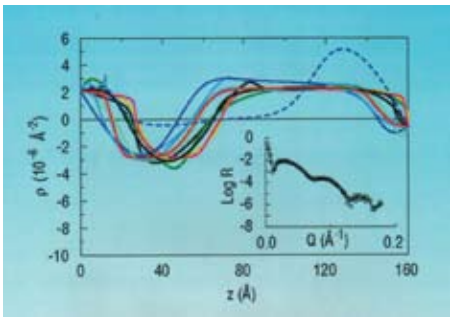


Figure 2. Family of scattering length density profiles (solid curves) resulting from a model-independent fit of the neutron reflectivity data shown in the inset [8]. The data are for a TiO/Ti film on silicon adjacent to an aqueous reservoir in an electrochemical cell [9]. The differences between individual members of the family are indicative of the uncertainty in the data associated with truncation of the reflectivity measurements at a finite maximum value of Q and from statistical fluctuations. The fits to the reflectivity are also plotted. The dashed curve is a single member of another, symmetry-related SLD profile that fits the data equally well. This is an illustration of the ambiguity arising from a lack of phase information, as discussed in the text. (After figures 5 and 6 of [8].)

A Brief History: In this section a partial chronology of neutron reflectometry development is briefly outlined. Given the scope of this article, it is not possible to acknowledge here, let alone adequately describe, all of the important work that so many people have contributed to the successful implementation of neutron reflectometry in many fields of scientific investigation.

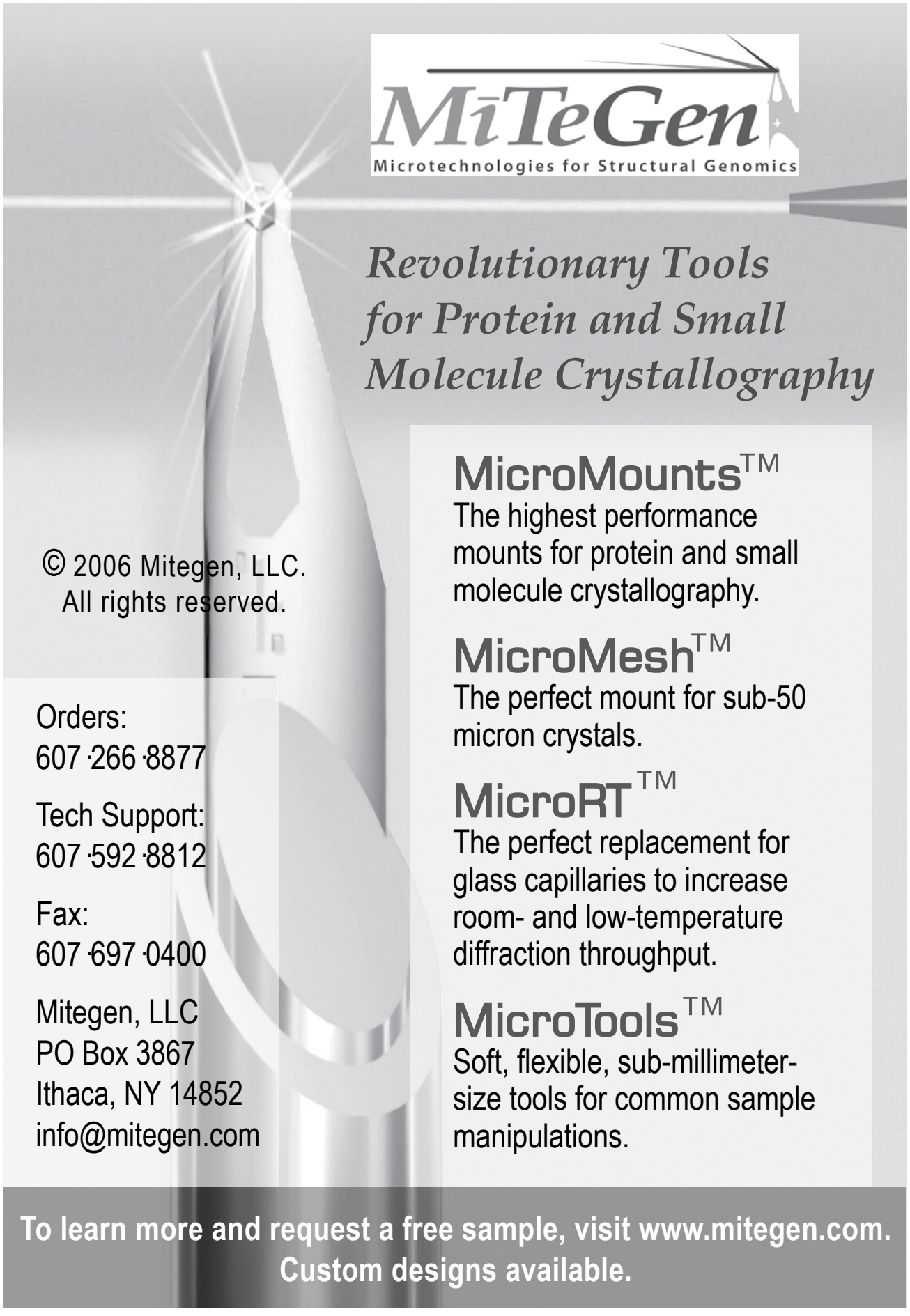
Beginning sometime in the mid 1980s and continuing through the early 1990s, Gian Felcher and company at Argonne National Laboratory performed some of the earliest pioneering NR measurements on magnetic and polymer thin films. Larry Passell, Feri Mezei and others developed highly efficient polarizing multilayers and supermirrors which were key to carrying out PNR studies of magnetic films and superlattices. Jim Rhyne et al. (at what was then NBS, now NIST) and collaborators at the University of Illinois and, independently, groups at Brookhaven National Laboratory and Bell Laboratories began studying magnetic interactions in rare earth superlattices (e.g., Dy/Y and Gd/Y) by polarized neutron reflection and diffraction. This early work [12] set the stage for later research on layered magnetic films that exhibit giant magnetoresistance which have technological importance in the reading of magnetic storage media. In soft condensed matter research, Steve White, among others, investigated biological membrane structures formed into multilayers suitable for neutron diffraction measurements. NR work began to emerge in other places around the world at about the same time, for example in the neutron scattering group at the Saclay facility in France and in Japan where an interest in magnetic multilayers was also growing. In Great Britain, Bob Thomas, Adrian Rennie, Jeff Penfold and others demonstrated the power of NR in studying organic systems, such as surfactants. At NIST, John Ankner performed some of the first grazing angle diffraction experiments with polarized neutrons. Meanwhile, Tom Russell et al. at IBM (now at the University of Massachusetts), and Frank Bates et al. at the University of Minnesota, initiated work with researchers at NIST and Argonne which explored new applications of NR to study diblock copolymer film systems. At this time an awareness of the significant problem that loss of phase information can cause in obtaining unique SLD profiles was becoming more widely recognized [13].

In the mid 1990s, a solution to the phase problem in dynamical specular NR was discovered, thus making possible, in both principle and practice, a means to resolve ambiguous problems when other sufficient independent information is lacking. Kent Blasie and coworkers at U. Penn and Susan Krueger and colleagues at NIST extended studies on biological membranes beyond multilayer samples to single lipid bilayer films containing macromolecules, measuring reflectivities as low as 1.0 x 10^{-7} at wavevector transfers of 0.7 inverse Angstroms. A diverse range of applications were now being pursued including: more complicated polymer thin film systems and brushes (Mark Foster et al. and Sushil Satija et al.); giant magnetoresistance (Julie Borchers, Hartmut Zabel, Eric Fullerton, Andreas Schreyer et al.); measurements of the London penetration depth in superconducting thin films (Gian Felcher et al.); multicomponent magnetic multilayer systems (Philippe Mangin et al.); magnetic exchange bias (Mike Fitzsimmons et al.); and interdiffusion (Greg Smith et al.).

In the late 1990s and early part of this century, progress continued unabated. Kevin O'Donovan and company introduced "front/back" measurement techniques in PNR for enhanced sensitivity in the study of noncollinear moment configurations in magnetic thin films. The groups of Roger Cowley, Hartmut Zabel, Henryk Kepa among others continued detailed, quantitative PNR investigations of magnetic single crystalline superlattices. Bjorgvin Hjorvarsson and Joe Dura et al. initiated a series of NR studies on the effect of H on the magnetic behavior of Fe/V superlattices. NR instruments were installed at nearly all neutron scattering facilities around the world and dedicated programs were launched.

Practical Scientific Applications: The aim of this section is to provide a representative selection, neither comprehensive nor all-inclusive, of illustrative examples of the application of NR in various fields of current research. Examples have been chosen largely on the basis that they cover a broader diversity of scientific areas and have a greater degree of first-hand knowledge about a particular experiment. The interested reader should have no difficulty finding numerous additional examples in the literature of NR studies in many fields of research.

One of the primary applications of neutron reflectometry in "hard" condensed matter has been the study of magnetic thin films and superlattices. Early polarized diffraction (PND) measurements on single crystalline superlattices composed of alternating layers of ferromagnetic Gd and nonmagnetic Y revealed either parallel or antiparallel coupling between successive Gd layers (each Gd layer composed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of a specific number, e.g., 10, of ferromagnetic atomic planes), depending upon the thickness of the intervening Y layer [14]. This effect was the first time such behavior had been observed in an artificially layered material and was explained in terms of a long-range, indirect exchange interaction (RKKY), mediated by the conduction electrons in the Y layers. According to this theory, the strength and algebraic sign (indicative of either parallel or antiparallel coupling) of the effective interaction between neighboring Gd layers varies in a decreasing and oscillatory manner, respectively, with increasing Y layer thickness. In this particular study, the superlattice reflections were measured about a Bragg reflection from the basal planes of the hcp Gd crystal structure; these satellites also appear, of course, about the origin at low Q and can be measured there as well. Even greater sensitivity to the vectorial magnetization structure can be obtained for noncollinear moment arrangements by measuring reflectivity curves with polarized neutron beams incident from both sides of the film [15] as shown in Figure 3.

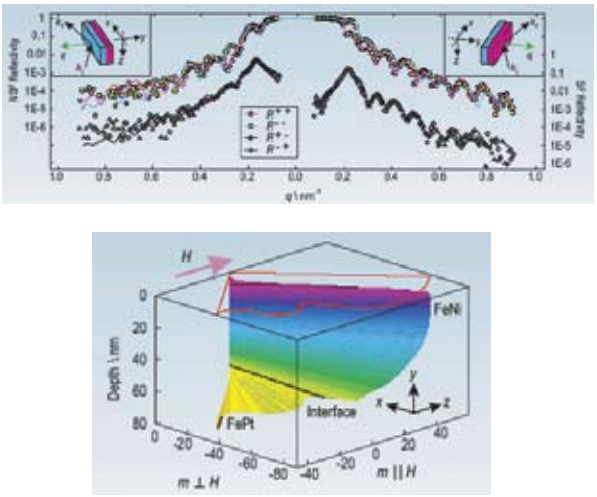

Figure 3. Upper part of the Figure shows PNR data collected with the incident beam intercepting the sample film from the front and back (i.e., from within the substrate) [15]. As described in the text, the combination of the two sets of data provides additional sensitivity in determining the vectorial magnetization depth profile in noncollinear systems. The lower part of the Figure is the magnetization depth profile that is obtained from the reflectivity above and corresponds to an FeNi/FePt layer sandwich .

An almost limitless number of superlattice combinations of magnetic and other intervening layer materials, e.g. a superconducting layer with a competing electron order parameter, can be imagined for designing systematic investigations, both fundamental and applied, of many material properties, as mentioned in the *Introduction*. Figure 4 shows polarized neutron, low-Q reflectivity and high-Q diffraction scattering data for an Fe/Cr superlattice [16] which can be combined to obtain a comprehensive and detailed picture of a complicated multicomponent magnetic system. Figure 5 shows detailed PNR data for a EuTe/PbTe system which is of particular interest for understanding semiconducting magnetic materials that are of potential importance in spin-dependent electronics technology [17]. In Fe/V multilayers studied by PNR, the magnetic behavior of the iron layers displays a remarkable sensitivity to the addition of relatively small concentrations of hydrogen in the vanadium layers [18].

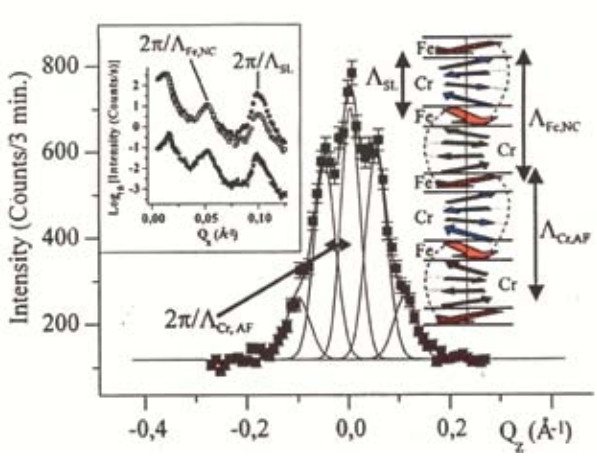

Figure 4. Low-Q PNR data (inset) and high-Q PND data from an Fe/Cr superlattice [16]. From this combined neutron scattering data, a detailed picture of the magnetic structure can be obtained. The relative orientation of neighboring ferromagnetic Fe slabs, each slab itself consisting of a discrete number of ferromagnetic atomic planes, is deduced principally from the low-Q reflectivity whereas the atomic scale configuration of the Cr moments in the intervening slabs is evident primarily in the high-Q diffraction data.

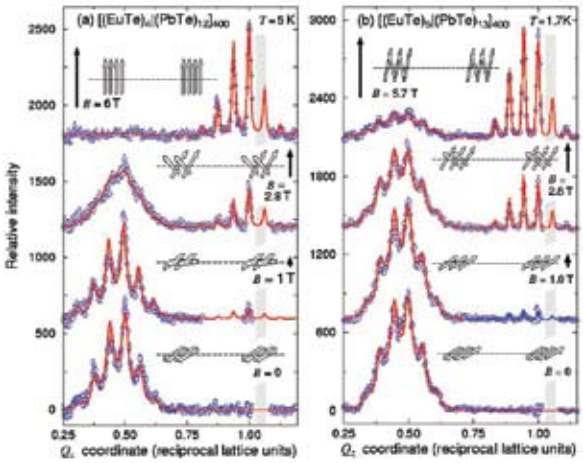

Figure 5. Another example of the detailed magnetic structural information that can be obtained by neutron scattering from superlattices [17].

In the examples presented above, PNR and PND provide exquisitely detailed structural information not directly obtainable by non-scattering means. In another application related to spin-dependent electronics, specular NR has been employed to study the spatial depth dependence of nuclear polarization reported to be induced in GaAs films when illuminated by circularly polarized light. The nuclear polarization occurs, in turn, through a hyperfine interaction between the nuclear magnetic moments and the electron currents polarized by the light. The neutron reflectivity is sensitive to the alignment of the nuclear spin be-

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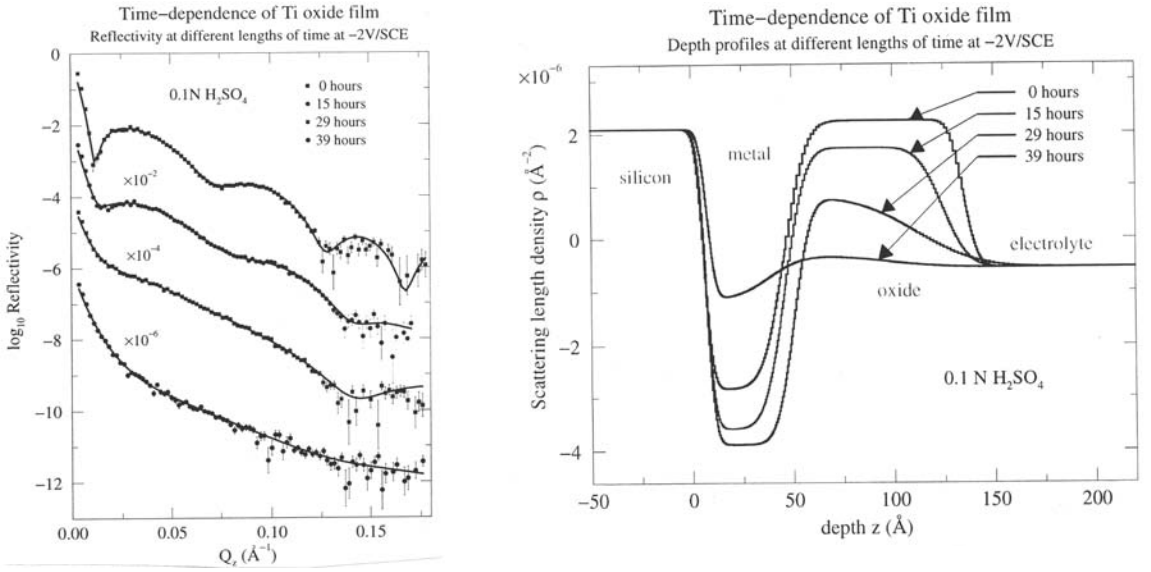

Figure 6. Specular neutron reflectivity data for a TiO/Ti film in contact with an aqueous reservoir under different electrochemical potentials on the left, corresponding SLD profiles to the right [9]. The measurements show how the corrosion process progresses with near nanometer spatial resolution.

cause the neutron-nucleus interaction is spin-dependent for nuclei with nonzero spin. Recent PNR measurements [19] indicate a depletion layer at the surface wherein the nuclear polarization is significantly suppressed.

Figure 6 shows the time dependence of the growth of an oxide layer on a titanium film as measured by NR *in situ*, in an operating electrochemical cell in which perfect single crystalline silicon serves not only as the substrate supporting the film but as the incident medium for the neutron beam [9]. This particular study also served as an example of the potential for ambiguous results due to a loss of phase information, as discussed earlier. However, in this particular case, one of two mathematically possible solutions could be eliminated based on the nonphysical magnitudes of the SLD in the constituent layers. Note the near-nanometer spatial resolution that is achieved in the chemical depth profiles determined as a function of electrochemical potential.

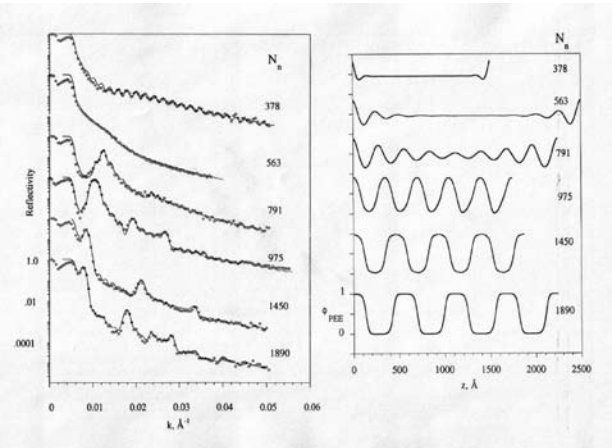

Figure 7. Specular NR data for several different PEP-PEE chain lengths on the left along with fitted curves corresponding to the SLD depth profiles on the right as discussed in the text [20]. The relatively large SLD difference between the two polymer constituents of the diblock is obtained by selective deuteration.

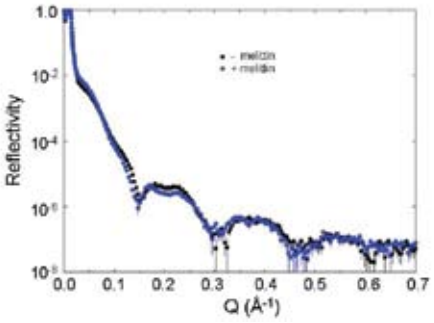

Figure 8. Neutron reflectivity data for a single lipid bilayer with and without melittin embedded in the upper phospholipid layer [22].

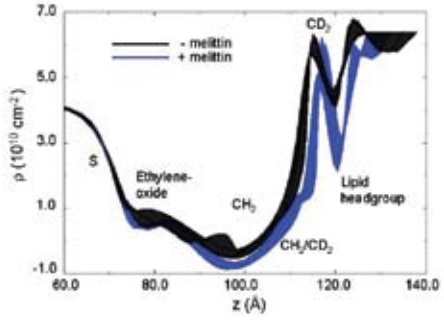

Figure 9. SLD depth profiles corresponding to the neutron reflectivity data of Figure 8 as described in the text [22]. The thickness of each of the continuous lines which indicate the magnitude of the SLD is indicative of the uncertainty in its value at a given point.

In soft condensed matter, NR has found wide applicability in the areas of polymer science and biology. Once again, the ability to substitute deuterium for hydrogen makes NR an extraordinarily sensitive probe of organic materials.

For example, NR can reveal how the presence of symmetry breaking interfaces affect the microstructure of systems that can undergo order-disorder transitions (ODT) [20]. Figure 7 shows NR data and corresponding depth profiles for a diblock copolymer consisting of a pair of different species, poly(ethylene-propylene)-poly(ethylethylene) (PEP-PEE), deposited on a silicon substrate. The development of a highly oriented lamellar morphology is clearly evident across the ODT.

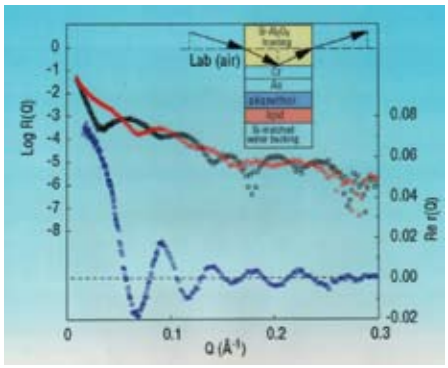

Figure 10. NR data sets (upper two curves) corresponding to two different composite layer systems having a common set of layers, Cr/Au/alkane thiol/lipid, but each composite possessing either a Si or Al_2O_3 substrate which serves as the "fronting" medium through which the neutron beam is incident [23]. Analysis of the two composite reflectivity data sets yields the real part of the reflection amplitude for the Cr/Au/alkane thiol/lipid layer sandwich of interest alone (lower curve). See text for discussion.

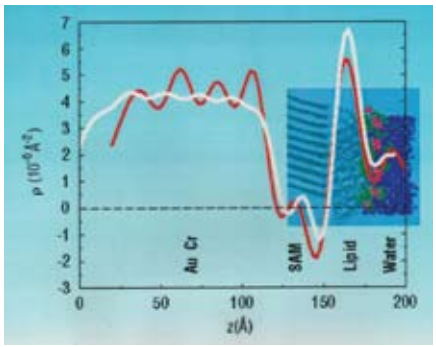

Figure 11. SLD depth profile (curve with the more pronounced oscillations in the Au region) obtained from the real part of the reflection amplitude appearing in Figure 10 by direct, first-principles inversion, as described in the text [23]. The nonphysical oscillations in SLD across the uniform Au layer are an artifact caused primarily by the truncation of the reflectivity data at a finite maximum value of Q. The other curve in the Figure is for comparison and represents the SLD for this bilayer system as predicted by a molecular dynamics simulation.

Neutron diffraction studies of lipid multi-bilayers have, over time, become an established means for extracting structural details from biologically relevant membranes [21]. More recently it has become feasible to investigate single lipid bilayers on flat support substrates by NR [22]. Figure 8 shows NR data sets for a hybrid bilayer membrane with and without the peptide melittin embedded. Plotting the same reflectivity data over a truncated Q range, multiplied by Q to the fourth power to compensate for the rapid Fresnel fall-off of the reflectivity from substrates with an abrupt edge, accentuates what are actually marked differences between the case without and that with the melittin present. Figure 9 shows the SLD profiles obtained by fitting the measured reflectivity data of Figure 8. The results indicate that the melittin is primarily embedded in the vicinity of the head group of the upper phospholipid layer. To gain further confidence in the SLD profiles so determined, given the phase problem discussed earlier, a set of phase-sensitive NR measurements on the same bilayer system without the melittin were performed by variation of the fronting medium [23]. A first-principles, exact inversion of these data, shown in Figure 10 along with the real part of the reflection amplitude corresponding to the Au and lipid bilayer films of interest, directly produced the SLD profile of Figure 11, in which a comparison to the SLD predicted by a molecular dynamics simulation is made (the oscillations in the uniform Au layer are an artifact intrinsic to the noninfinite reflectivity data set truncated at the maximum value of Q which could be attained in the experiment).

Future Advances: Not surprisingly, obtaining higher intensity neutron sources is always a top priority for advancing scattering techniques. The new Spallation Neutron Source (SNS) at Oak Ridge National Laboratory is a major step in this direction. Recently, two state-of-the-art neutron reflectometers have been brought on line there. At pulsed sources such as the SNS, ISIS in the UK or LANSCE at Los Alamos, specular NR is performed with a wide spectrum of the wavelengths present in a given pulse since a specific wavelength component associated with a particular Q can be identified via time of flight. At continuous, reactor-based sources, monochromatic beams are frequently utilized in NR. This is highly inefficient and efforts are currently underway to address this deficiency. For example, at NIST one plan being considered employs polychromatic, continuous incident beams. Wavelength analysis of the specularly reflected beams then would be performed via wavelength-sensitive Bragg reflection from an array of single crystal analyzers.

The use of relaxed angular divergence along one of the sample's in-plane directions results in a significant intensity increase for specular measurements with negligible loss of resolution for Q perpendicular to the surface. However, the price paid for this relaxed angular collimation is a marked degradation of the in-plane resolution in the corresponding direction. Obtaining good resolution in two orthogonal in-plane directions without prohibitive losses in intensity requires that a divergent beam still be employed in at least one direction but with angular information encoded by another means, such as labeling the angle of a given trajectory by neutron polarization direction. This latter method has been explored recently by a number of different groups (including those of Pynn, Felcher, Rekveldt, and Major[24]).

Finally, just as the ability to create single crystalline superlattices and other multilayers has made, and continues to make possible a wide variety of NR, PNR, and PND studies of hard and soft condensed matter systems. The progression to surface-patterned films and multilayers literally adds another dimension to the range of potential systems which can be investigated in the future.

Acknowledgements: The development of neutron reflectometry has progressed because of the concerted efforts of many individuals working in various groups around the world. For the scientific research highlighted by the examples in this article, credit is due in particular to my colleagues, past and present, and to the NIST Center of Neutron Research for its generous and steady support.

Charles F.Majkrzak

Center for Neutron Research - National Institute of Standards and Technology

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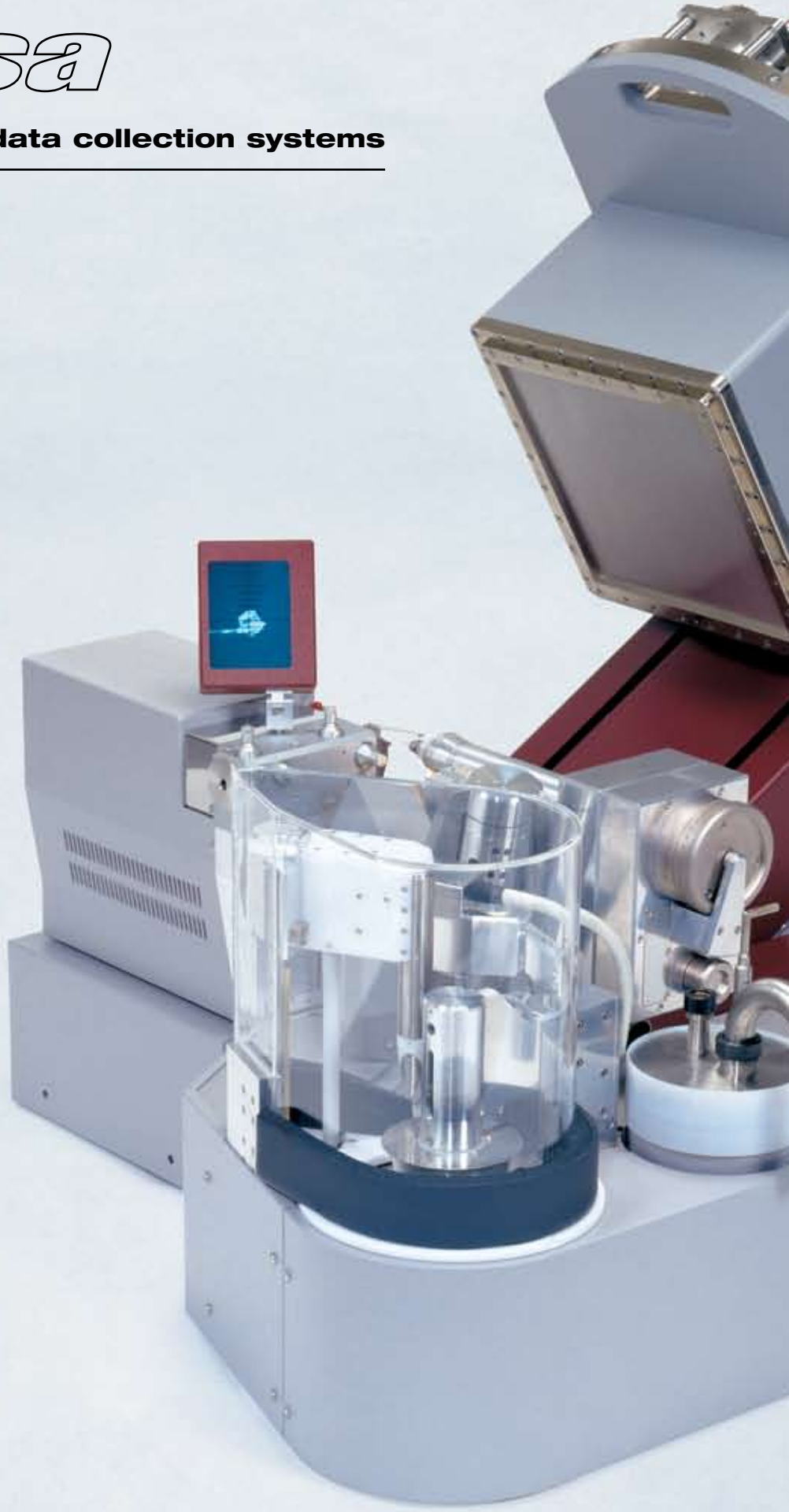

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Candidates for ACA offices in 2008

The Nominating Committee (*Brian Toby (Chair), Bob Bau and Jeanette Krause*) has proposed the following candidates for the 2007 elections for ACA offices in 2008

Vice-President: **Robert VonDreele and Winnie Wong-Ng**

Canadian Reprsentative to Council: **Jim Britten and Mirek Cygler**

***Committees*:**

Communicatons: **Allen Oliver and Thomas Proffen**

Data, Standards & Computing: **John Faber and David Harrison**

Continuing Education: **Cora Lind and Peter Mueller**

To nominate write-in candidates for any of these offices, write to the ACA Secretary: Lisa J. Keefe, IMCA-CAT, Sector 17, Bldg. #435A, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439. (Fax: (630) 252 0521) Letters must be received by September 15, 2007 and must be signed by 5 supporting ACA members and include a signed statment by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in October 2007

Robert B. Von Dreele
Vice-President

Senior Physicist, Argonne National Laboratory; joint appointment with the Intense Pulsed Neutron Source (IPNS) as Instrument Scientist for the Special Environment Powder Diffractometer (SEPD) and the Advanced Photon Source (APS) in the Materials Characterization Group of the X-ray Science Division.

Education: BS Chemical Engineering, Cornell . (1966); PhD Chemistry, Cornell (1971), advisor R. C. Fay, NSF Postdoc Fellow, Inorganic Chemistry, Oxford. (1972-73) with J. S. Anderson.

Professional Activities: Professor of Chemistry, Arizona State University (1971-1986) and Staff Member, Los Alamos National Lab (1986-2003) in the Manuel Lujan Neutron Scattering Center and Instrument Scientist for the High Intensity Powder Diffractometer (HIPD). Fulbright Scholar at the ISIS Facility, Rutherford-Appleton Laboratory (1986). Fellow of the Mineralogical Society of America (2001); Member of the U.S. National Committee for Crystallography (2007-present); Member International Union for Crystallography Commission for Powder Diffraction (1996-2002); Technical Manager for High Pressure/Preferred Orientation (HIPPO) diffractometer at LANSCE (1999-2002); team member for development of dedicated high resolution x-ray powder diffractometer on 11BM at APS (2002-present); principal developer of the General Structure Analysis System (GSAS) (1984-present); member DOE Mid-Scale Instrumentation Review Panel (2007); chair of IPNS Elastic Scattering Proposal Advisory Committee (2006-present); visiting staff member, Los Alamos National Lab, (summers 1980-1984).

Research Interests: My interest in crystallography began as a graduate student at Cornell, in the midst of thesis work on synthetic inorganic chemistry, by doing a heavy atom determination of a 7-coordinate complex of zirconium using film techniques along with structure determinations of a complex oxide and a moderate sized natural product with diffractometer data in the crystallographic laboratory of Lynn Hoard and Bob Hughes. The whole idea that one could get this very visual and detailed picture of atomic arrangement from diffraction was very exciting and very satisfying to me. My introduction to neutron powder diffraction came during my postdoc at Oxford University when Tony Cheetham and I hooked up to try it out using Hugo Rietveld's new computer program. It was clear to me that this was the most exciting and challenging problem in crystallography - getting the most out of a powder pattern. This led to my beginning to try to use x-ray powder data (later embodied in the Wiles & Young program, DBWS, the ancestor of FULLPROF, and many other Rietveld refinement programs) and the first practical application of the Rietveld Method to neutron Time-of-Flight (TOF) data. In the 1980's Allen Larson and I collaborated to produce the now very well known GSAS package; this has given me a platform to further develop powder diffraction for profile shapes, preferred orientation (texture) and even for protein structure analyses and then let the community make use of them in their work. Protein work forms the core of my present scientific interest and is arguably the ultimate challenge - to solve a protein structure from powder diffraction data.

Statement: I am humbled and flattered to be asked to follow in the footsteps of the giants of our community and be nominated as a candidate for the Vice-President of the ACA. I've been a member of the ACA since joining as a graduate student in the early 70's and it has been the one professional society with the broadest coverage of the science of crystallography. In that time crystallography has changed dramatically from the time when doing a crystal structure or two could suffice for a publication or even a thesis project to what is now a "technique" on a par with the various spectroscopies commonly available in a chemistry laboratory. This change has been driven by developments in instrumentation and more especially by extreme improvements in computational power and software so that most crystal-

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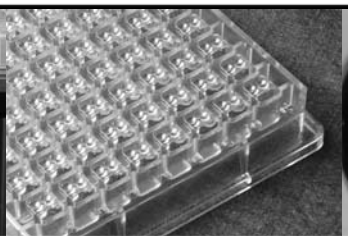
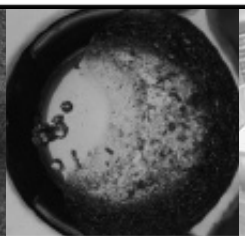


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lographic structure determinations can now be performed in a "black box" mode with very little human intervention. Even protein structure determination has succumbed to this drive toward automation. While this has been happening for single crystal crystallography, powder diffraction has been transformed all out of recognition from a qualitative/quantitative phase analysis tool done largely in industrial laboratories to a very powerful structural probe usable under extreme conditions on samples that do not normally exist as single crystals. The scope of powder diffraction is rapidly expanding and even proteins are not out of bounds. Moreover, powder diffraction is now used to address bulk properties such as stress/strain and texture in polycrystalline objects which is of great interest to ceramicists, geologists and metallurgists. We have also seen the development of dedicated user facilities in neutron and x-ray scattering constructed at national laboratories that provide brilliant sources and exceptional instrumentation. The explosion of crystallographic information that has resulted from all this is truly staggering; with almost 50,000 protein structures in the PDB, over 400,000 structures in the CCDC, and over 250,000 entries in the PDF-4+ powder diffraction file offered by ICDD.

Now the bad news: crystallography is a dying discipline in many universities; many chemistry, physics and geology departments do not have (or want) faculty whose research is driven by a basic grounding in crystallography. The common choice is to relegate crystal structure determinations to departmental staff or else have structures done by mail order. While this does "get the job done" for routine structure determination, the loss is that training in basic crystallography for graduate students and postdocs becomes very spotty at best and completely absent in many locales. I recently saw in the MSA e-mail list many comments from mineralogists about this loss from geology and in some cases describing the complete obliteration of the discipline at their university. Is this a dead end for crystallography?

As I'm sure you know, I develop and maintain a significant crystallographic computer program (GSAS). In fact, I interrupted my work on this statement to chase down a user reported bug! Much crystallographic software was originally written many years ago by a very small number of folks who had essentially taken this up as a "hobby" and, in one way or another, let the larger community use the fruits of their labors. These codes are commonly in FORTRAN and are becoming more difficult to maintain as that expertise dies. We now want our software to be GUI based and easy to use "black boxes" which requires that all of the accumulated crystallographic "tricks" be somehow coded into them. This requires a new combination of crystallographic and software engineering talents that may be hard to come by.

To meet these challenges, I believe the ACA needs to continue to have an active role in encouraging the development of new ways of providing training and education in crystallography through workshops, summer courses, web-based courses and, of course, the program offered at our annual meeting. Perhaps we can learn from the experience of the Rietveld e-mail list where questions (and sometimes contentious comments) are posted by list members about powder diffraction; students in particular almost always receive helpful replies from others. We should have something like this for all of crystallography where e-mail list membership is automatically offered to all ACA members.

In my own particular path through crystallography, I have increasingly become very impressed with the wide variety of tools and techniques that have been developed by the various parts of our community to aid in solving the central problems of crystallography. However, I suspect that much of this knowledge gained in one corner of our science remains unknown and unavailable to the others. The role of the ACA should be to be sure that cross-fertilization occurs between the various subdisciplines within crystallography so that all of us can benefit from this hard-won knowledge. I would encourage future program chairs for our annual meetings to find ways for our various disciplines to "mix it up" so we can learn from each other as well as encourage participation (especially by students!) from all corners of crystallography. In my own experience there are incredible scientific riches in the spaces between our various disciplines and the ACA should be there to help us find them.

Winnie Wong-Ng
Vice-President

Senior Research Scientist, Ceramics Division, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, A256 MATLS, 100 Bureau Drive, Mail Stop 8520, Gaithersburg, MD 20899.

Education: BSc, Chemistry, Chinese University of Hong Kong (1969). PhD, Inorganic Chemistry, Louisiana State University (1974) with Steve Watkins; Postdoctoral fellow/Research Associate/Lecturer in Chemistry Department, University of Toronto, Canada, with Stan Nyburg.

Professional Activities: Local chair, 1998 ACA annual meeting, Arlington, VA; chair/member, ACA Continuing Education Committee (2001-2003); secretary/treasurer, US National Committee for Crystallography (USNCCr, 2000-2003); chair, ACA Warren Award Committee (2005); chair/member: ACA Nominating Committee (2002-2003); co-organizer of four ACA scientific sessions (1989, 1992, 1993, 1998); co-organizer of more than 20 symposia/workshops at various other scientific meetings; chair, Membership Committee, International Centre for Diffraction Data (ICDD, 2001-2004); chair, Ceramics Subcommittee, ICDD (1994-2000); member, ICDD Awards and Scholarship Committees (2004-present); chair, thermoelectric task group, ICDD (2006-present); chair, high-temperature superconductor task group (1994-present); chair, Electronics Division, American Ceramic Society (2005-2006); member, Board of Directors, Applied Supercon-

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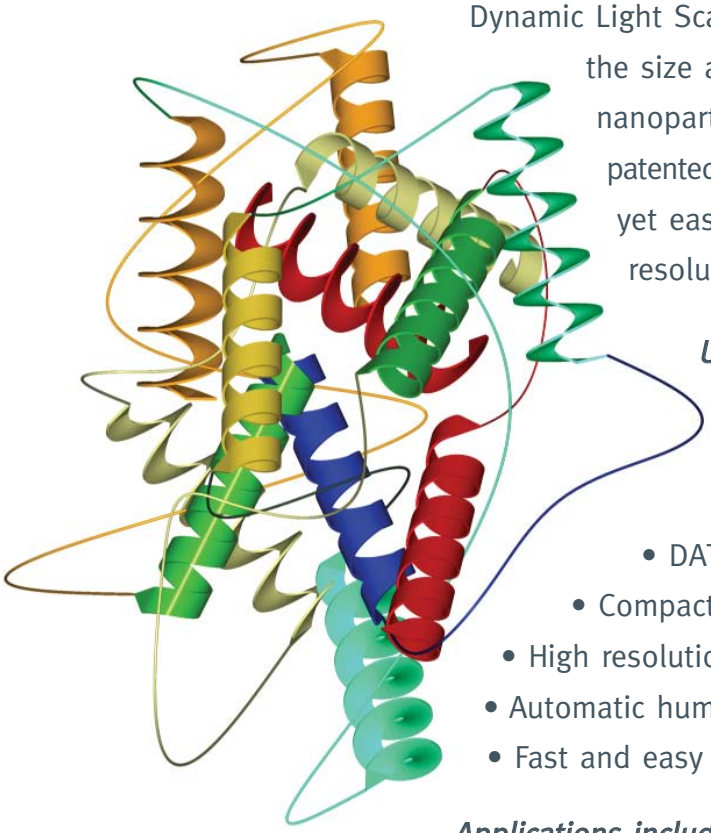

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ductivity Conference (ASC), 2007; editor, international report section of *Powder Diffraction* (1999 - present); guest co-editor, special issue of *J. Research of NIST* (2001); guest co-editor, special issue of *J. American Ceramic Society* (2008); *Honors and Awards*: Fellow of ICDD (2001); Fellow of American Ceramic Society (2002); recipient of the Bronze Medal for superconductivity research from Department of Commerce (2002); recipient of the McMurdie Award for significant contribution to the Powder Diffraction File (2004); about 250 publications.

Research Interests: Crystallography, crystal chemistry, phase equilibria, structure/property relationships of high temperature materials including complex oxides; standard reference materials; reference x-ray powder patterns/data; databases; single crystal and powder diffraction crystallography (x-ray, neutron, and electron); high-temperature and high-pressure x-ray diffraction; modeling; superconductors; thermoelectric materials and other energy-related materials; fast-throughput combinatorial thin film metrology.

Statement: I am very honored and proud to be a candidate for election as the Vice-president of the American Crystallographic Association. The ACA is the first scientific organization that I joined when I was a graduate student. Needless to say, I am extremely delighted to have this possibility to serve the organization that I care about, respect, and 'grew up' with.

Having worked at the University of Toronto, the International Centre for Diffraction Data, and the Material Science and Engineering Laboratory of NIST for more than a combined total of 30 years, I have been very fortunate to have had the opportunity to work on a great number of structural science-related projects. I believe I can bring to this office an appreciation for the diverse fields of crystallography that I have been interested or involved in. I truly recognize the impact an organization such as the ACA can have on its members' everyday crystallographic research activities.

The vice president position comes with many key responsibilities. As your vice-president, I will use my experience as the 1998 ACA local chair and my extensive experience as a symposium organizer to ensure the success of our annual meetings. I will use my experience as the secretary/treasurer for the USNCCr to serve as an ACA representative to USNCCr. I will use my experience as the Chair of the Ceramics Division of the American Ceramic Society, as the President of the Association of NIST Asian Pacific Americans, and as a member of the BOD of ASC to assist the ACA president in making important policy decisions for ACA, and to serve as a knowledgable member of the ACA council. As the ACA plans its strategies and growth for the years ahead, I would like to contribute my views concerning the following activities.

I believe it is the duty of the ACA council to be an advocate for various structural research areas. While maintaining the health and growth of the macromolecular crystallographic component of the organization, we also need to advocate and build up the strength of the components that are related to small molecule research, including minerals and materials that are of state-of-the-art technological importance. In this way, the harmony between the macro- and small-molecule components of the ACA could be extended to a higher level.

One way to achieve the growth of an organization is through focused membership drives. New members will provide us with new scientific insights and resources. Therefore we need to design strategies to gain new members. There are many scientists who have crystallographic knowledge and are currently participating in other scientific societies, but they are not members of the ACA. Many of these societies may also have interests in structural science or the crystalline state. We need to cooperate with these organizations to identify potential new members, to ensure that structural data is appreciated, and to raise the profile of our organization. We need to provide potential new members with effective opportunities to join us. The form of cooperation between societies could include joint symposia/sessions, cross-links on the world-wide web, or even mutual access of membership rosters. We also need to expand membership among our industrial colleagues. Industrial crystallography could be an important component of the association.

With the help of our SIGs, we must strive to build a strong and balanced scientific program during the annual meetings that will meet the needs of our members as well as attract new members. The program should include state-of-the art techniques, theory, software, and materials of current technological interest. During these meetings, we should take the opportunity to increase our visibility by contacting the scientific press to showcase our publications and programs. We should also strengthen the special transaction symposia and plenary lectures to reflect state-of-the-art crystallographic research.

With the advent of modern computer technology, in addition to the creation of macromolecular information from high throughput techniques, a vast volume of other diffraction data will soon be available due to the increasing importance of the combinatorial approach in materials research, an area that I am also currently involved in. To be able to access this large volume of diffraction data, various computational strategies and standards are critical for data collection, storage, transport and exchange. Communication and cooperation between creators/producers of crystallographic databases and those responsible for other property databases are important in order to maximize research opportunities for all. We should emphasize the potential of a combined use of these databases for maximizing their impact.

Crystallographic education is extremely important for our institutional health. We must continue to provide training opportunities for our young members as well as for our more established professionals. It is our responsibility to ensure the strength and skills of the next generation of crystallographers by providing them with the necessary education. We will strive to increase resources for supporting attendance of more young people at ACA annual meetings. We will investigate possible ways of establishing scholarships for crystallographic studies. We will make sure our annual meeting program will continue to meet the needs of our members by providing ample networking opportunities and mentoring by senior members. We must also continue to support and encourage the ACA for the macromolecular and small molecule summer schools.

I believe a well-planned outreach program is important for the growth and visibility of our organization. In addition to continuing to support research and edu-

cation, and to meet the needs of the membership, we need to increase our outreach to Central and South America. We should also facilitate educational opportunities for the public in general, for example, by encouraging our members to give talks about crystallography at local high schools. We can also encourage teachers from local schools to teach crystallography by inviting them to attend selected sessions on crystallographic education during the annual meetings.

If possible, the ACA should make available the information from science policy makers to the crystallographic community. We should establish efforts to help influence public policy, particularly as related to the support of national resources such as the synchrotron, neutron and electron research facilities, as they are vitally important to many of our members. We will investigate the possible creation of a mechanism to bring the members' concerns to the attention of the policy makers. We should also support efforts to increase public funding of all components of crystallographic research.

Good communication is one of the main keys to success in every organization. I will encourage increased communications between the council and the ACA members. I will welcome all suggestions and comments from the members. Those comments or discussions concerning important issues will be shared in ACA *RefleXions*.

If honored with your election, I pledge to commit my best efforts to fulfilling the responsibilities of the office. I will apply the experience that I have gained in working at academic, industrial and government institutions to serve the ACA by following up on important opportunities and issues. I will ensure the continuous prosperity and growth of the organization, and the steadfast advancement of the field of both macromolecule and small molecule crystallography.

Cora Lind
Continuing Education

Assistant Professor, Department of Chemistry, University of Toledo, Toledo, OH.

Education: Prediploma, 1996, Bergische Universität Wuppertal; MS 1999, PhD, 2001, Georgia Institute of Technology.

Professional Activities: Postdoctoral associate, 2001-2003; Cornell, session organizer Gordon conference 2006; ACA Margaret C. Etter Early Career Award 2007; NSF career grant (***www.chem.utoledo.edu/FAC_INFO/Lind/SOURCE.htm***).

Research Interests: Structure-property relationships in solid-state materials, x-ray and neutron powder diffraction, Rietveld analysis, structure determination from powder data, non-ambient diffraction (low+high temperature, high pressure), phase transformations as a function of temperature, pressure and composition.

Statement: Structural characterization of materials is important for many aspects of scientific research. With the advancement of hard- and software, structure solution is no longer restricted to small molecule single crystal diffraction. It is now widely accepted that structures can be determined for macromolecules and powder samples. At the same time, I frequently encounter powder diffractometer users that have a very biased view of the information that they can extract from their data. At the two extremes, this ranges from limiting themselves to phase identification by searching a database, to users that demand that I show them how to solve the atomic level structure of their poor quality powder data within half an hour. What both sides are lacking is a solid crystallographic background that allows them to make an educated judgment on what kind of knowledge they ***can*** gain through a specific experiment - and on how to set up their experiment properly to get reliable data. Many of them never considered crystallography as an integral part of their education. As a member of this committee, it would be my goal to reach out to researchers who would not traditionally consider themselves crystallographers, to educate them through courses, lectures and workshops about the opportunities and limitations of a variety of experiments ranging from single crystal to powder diffraction.

Peter Mueller
Continuing Education

Director, X-Ray Diffraction Facility, Massachusetts Institute of Technology, Cambridge, MA 02139, pmueller@mit.edu.

Education: Vordiplom (BA equivalent) Chemistry, University of Kaiserslautern, Germany (1994); PhD in Inorganic Chemistry/Crystallography with George Sheldrick, University of Göttingen, Germany (1997-2001); postdoctoral work in Molecular Biology with David Eisenberg, University of California Los Angeles (2001-2004).

Professional Activities: Research and teaching assistant in George Sheldrick's group (1997-2001); research associate / teaching fellow with David Eisenberg (2001-2004); director of x-Ray diffraction

facility and lecturer for crystallography at MIT (2004-present); regular reviewer for *Acta Cryst.*, *J. Am. Chem. Soc.*, NSF; Secretary/Treasurer of the ACA General Interest Group (2003-2006); chair of the ACA General Interest Group (2007); chair elect of the ACA Service Crystallography SIG (2007); session chair and organizer of ACA meeting sessions on Teaching Advanced Crystallography (2004), Data Collection Strategies (2005), Whole Molecule Disorder (2006), Teaching Gadgets (2007); organizer of the SHELX workshop at the 2007 ACA meeting; invited faculty at the ACA Small Molecule Summer Schools 2006 and 2007; organizer of an annual crystallographic symposium at MIT (past symposia 2005-2007); teacher of structure refinement and data reduction at workshops in Göttingen, Germany (1997 and 2003), College Station, TX (2000), Madison, WI (2003 and 2005), Cambridge, MA (2005, 2006, 2007); initiator and organizer of a workshop held at MIT for undergraduate chemistry students from the College of the Holy Cross in Worcester, MA (2006 and 2007); initiator of an outreach program and collaboration to include crystallography in the science education at the Philips Academy in Andover, MA; main author and editor of *Crystal Structure Refinement* (IUCr Texts on Crystallography number 8, Oxford University Press 2006).

Research Interests: Data collection strategies, refinement methods, whole molecule disorder, charge density.

Statement: X-Ray structure determination is a key method in the life sciences, chemistry, materials sciences and other disciplines and one would expect crystallography to be an important part of the education of every scientist working in those fields. Strangely, however, serious courses in crystallography cannot be found on many curricula. If crystallography is taught at all, it frequently is a marginal part of a physical chemistry class, and only a few hours are available to introduce the method. This is unfortunate, as a majority of scientists relying on crystal structures do not understand the method well enough to evaluate the results of or to draw their own conclusions from the crystallographic data. Basic crystallographic education could start as early as high school and should be taught to undergraduates. In any case, crystallography should be offered as an 18- to 24-unit course to all graduate students of the disciplines mentioned above. Together with the NSF, USNCCr, ACS and the IUCr's Teaching Commission, the ACA should play a prominent role in fostering crystallographic education at all levels and should help to establish basic teaching standards. I would work in this direction as a member of the Continuing Education Committee.

A different aspect of crystallographic education is the training of scientists who want to determine crystal structures not only occasionally and under the guidance of a trained crystallographer, but fully on their own. The training of a professional crystallographer reminds me of that of a Jedi knight: the practical knowledge only goes from the master's mouth to the apprentice's ear and it can be difficult for the outsider or autodidact to become adept without a local guru's help. At the same time, modern software has become so reliable that many routine structures can be determined without any skill other than the ability to repeatedly hit the carriage return key while simultaneously ignoring occasional error messages. To overcome this black box phenomenon is a key challenge for the ACA, and crystallographic education must continue well beyond the regular classes mentioned above. The annual ACA Summer Courses as well as workshops held at annual ACA meetings are important for the development of the crystallographic community, but I would like to see the ACA put an even higher emphasis on education. Several attempts to establish an Education Special Interest Group have failed in the past years. As the current chair of the General Interest Group I will try to amend the bylaws of this group to include an educational mandate. As a member of the Continuing Education Committee I would use my experience in organizing and teaching to work towards offering, promoting and sponsoring a broader range of workshops and courses and to make education one of the top priorities of the ACA.

John Faber

Data Standards and Computing

Principle Scientist and X-ray Clinic Technical Director, ICDD
Newtown Square, Pennsylvania

Education: Assoc. in Applied Science, DeVry Technical Institute, Chicago, IL, BEE and PhD at Marquette University, Milwaukee, WI.

Research Interests: My research interests span x-ray and neutron powder diffraction for materials research, including structure and properties of high temperature materials; the generation of powder diffraction patterns from structural data using on-the-fly technology; and design and use of relational databases for housing powder diffraction and structural data, especially using web-based client/server technology.

Professional Activitices and Statement: As ICDD's Principal Scientist, I have been responsible for creating and directing a team of specialists to develop new products based on relational database (RDB) technology. The technical initiatives include conversion from existing data structures, database design, security, licensing, and utilization of web-based e-commerce. I have worked on tools for rapid identification, total pattern analysis, and data mining. I have built major marketing and business ties with OEMs and 3rd party developers. My past experience includes employment at the University of Illinois at Chicago as the Associate Director of Research; Amoco Corporation as Associate Research Scientist and Senior Research Scientist; and Argonne National Laboratory as a Staff Scientist. I was elected Fellow of the ICDD in 2005. I would like to serve on the Data Standards and Computing Committee.

David Harrison
Data Standards and Computing

Education: BS, MS in chemistry from Emory University (1983); MPhil. in molecular biophysics and biochemistry from Yale University (1985); PhD in molecular biophysics and biochemistry from Yale University (1992).

Professional Activities: Computer programmer for Batterymarch Financial Management (Boston) during the summers 1978 – 1983; president and programmer of Down East Computing (Boston) 1985; protein engineer/crystallographer for Eastman Kodak (Rochester) 1986; Post-doctoral fellow with Greg Petsko and Dagmar Ringe at Brandeis University 1992-1995; assistant professor at the Medical College of Wisconsin (Biochemistry) 1995-2000; associate professor at the Medical College of Wisconsin (Biochemistry) 2000-2003; associate professor at the Rosalind Franklin University of Medicine & Science (Biochemistry and Molecular Biology) 2003-present.

Research Interests: I am interested in molecular recognition and catalysis by enzymes.

Statement: As the field of macromolecular x-ray crystallography becomes more like that of small molecule x-ray crystallography, it becomes more and more important that crystallographic data be able to stand on its own without the need to rely on accompanying publications. Data standards make it possible for automated bioinformatics programs to work on public databases without intervention by researchers and programmers. The two issues that I would focus on are data quality and data standardization. In college, I spent my summers doing database programming in FORTRAN for a financial management company. From this experience I gained a solid understanding of the nuts-and-bolts of database programming, which has given me insights into how data standards may ease database design. I also spent a short time as a small molecule crystallographer and I am aware how data standards have been used to allow systematic characterization of bond lengths, bond angles, and non-bonded interactions. I have also spent several years as a producer of macromolecular crystallographic data. I am aware of how important it is that the standards not unduly interfere with the process of model refinement and data deposition. Further, in light of recent events, it seems to me that standards must be adopted for the submission of experimental phases as well as the routine deposition of derivative and MAD datasets in addition to the deposition of native data. It should be possible for researchers to objectively view crystallographic data without model bias in the case of controversial publications. I look forward to the opportunity to work with the data, standards and computing committee.

Allen Oliver
Communications

Research Crystallographer, Department of Chemistry and Biochemistry, University of California Santa Cruz, Santa Cruz, CA 95064.

Education: BSc Chemistry, Waikato University (1992); MSc(hons) Chemistry, Waikato University (1994); DPhil Chemistry, Waikato University (2000); Postdoctoral fellow, University of California Berkeley (2000-2002).

Professional Activities: Member of the ACS, ACA and PDS; currently serving as chair for the Service SIG, chair-elect for the General Interest Group and secretary for the Small Molecule SIG within the ACA; secretary for the Pittsburgh Diffraction Society; reviewer for *Dalton Transactions*.

Research Interests: Chemical crystallography in a service environment; chemical crystallography at synchrotron sources.

Statement: I am honored to be nominated for election to the ACA Communications Committee. Communicating concepts, information and results are vital to any society; both within the society and to the public at large. Today's crystallographic research covers a diverse range of topics and we need to be able to present our ideas to those within and outside of our field of specialization. I would endeavor to work with the committee to promote more interdisciplinary discussions to strengthen our understanding of the fields within our chosen profession. Furthermore, I would endeavor to raise public awareness of the ACA and what we provide to the greater community.

Thomas Proffen
Communications

NPDF Instrument Scientist, Lujan Neutron Scattering Center, LANL, MS H805, Los Alamos, NM 87545.

Education: PhD in crystallography at the University of Munich, postdocs at the Australian National University and Michigan State University.

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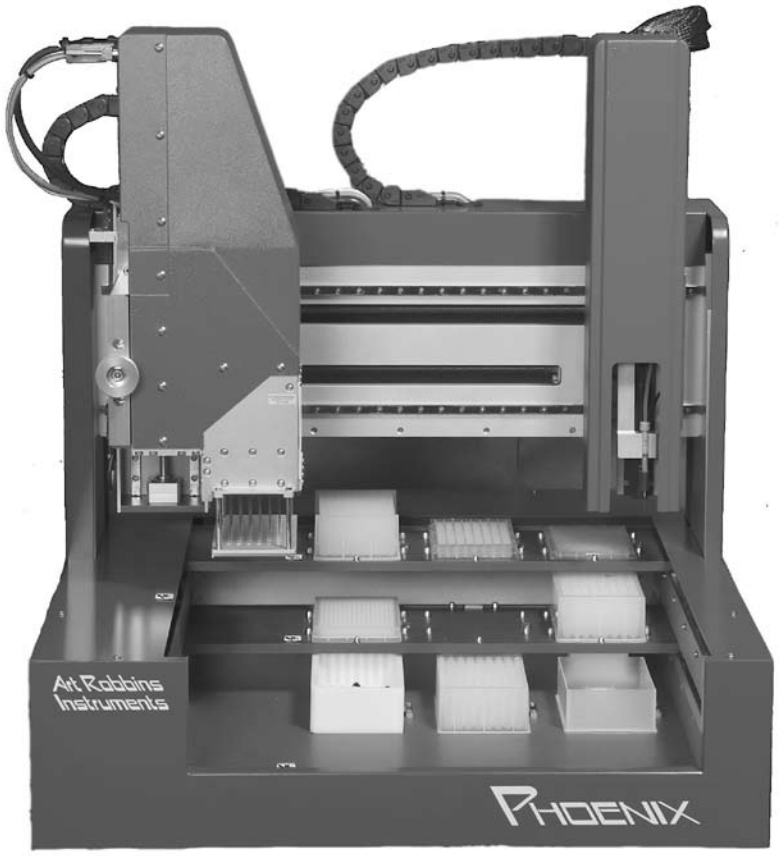

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Professional Activities: Co-editor for *Zeitschrift fur Kristallographie*, member of the executive committee of the instrument advisory team for the single crystal diffractometer TOPAZ under construction at the Spallation Neutron Source, past chair of the Neutron and current chair of the Powder Diffraction SIG.

Research interests: Study of disordered materials using total neutron and x-ray scattering applied to exotic oxides, geomaterials and more recently hydrogen storage materials. I started my career analyzing single crystal diffuse scattering from inorganic materials and over time became involved with atomic pair distribution function analysis to study similar disordered materials using powder diffraction. As an instrument scientist at NPDF at the Lujan Center, my technical interests include software development for data reduction and modeling as well as getting the PDF technique 'out there'.

Statement: Being a crystallographer (I indeed have a PhD in crystallography) by education, I jointed the ACA as soon as I came to the US about 8 years ago. One issue close to my heart is bringing a notion of what and how important crystallography is to the wider public, to schools and to the colleagues in the next building. On more than one occasion when asked my profession, my reply 'I am a crystallographer' resulted in being asked abou the healing powers of a particular stone, so there is a long way to go. I remember attending the IUCr meeting in Seattle and, in particular, listening to the panel discussion by several Nobel prize winners, all related to crystallography. Even I was impressed. I see the function of the ACA Communications Committee as key to providing a united voice to politicians, funding agencies and the public and, if elected, I will work as hard as I can to achieve these goals.

Jim Britten

Canadian Representative to ACA Council

Assistant Professor, Department of Chemistry and Brockhouse Institute for Materials Research, Manager, MAX Diffraction Facility, McMaster University, Hamilton, ON, Canada L8S 4M1.

Education: BSc St.Francis Xavier Univ. (1977); PhD McMaster U. (1984); postdocs NSERC , U. de Montreal (1984,1985) and Killam, Dalhousie U. (1986).

Professional Activities: Vice-chair, Canadian Nat. Comm. for Crystallography; member of Beamline Advisory Committee, CLS; reviewer for *J. Chem. Cryst.*; secretary, ACA Canadian Division (1998,1999), chair (2003-2006); co-organizer of ACA 2007 *Transactions* Symposium on "Diffuse Scattering"; co-organizer of "Laboratory X-Ray and Neutron Diffraction for Materials Chemistry" for 2007 CSC, Winnipeg; co-organizer of session "Canadian Light Source" at ACA2006; chair, Service SIG, ACA, 1997; organizer of session on "Service Crystallography at Synchrotrons", ACA 2000; member of Canadian Institute for Synchrotron Radiation; principal investigator for small molecule crystallography beamline proposal (approved) at the CLS; member of the beamline team for the Brockhouse scattering and diffraction sector at the CLS.

Research Interests: Molecular and solid state crystallography; reciprocal space volumes; diffuse scattering; 2D and 3D powder diffraction of alloys, films, and polymers; synchrotron crystallography; crystallographic education; charge density

Statement: It is an honor to have been nominated as a candidate for Canadian Representative to ACA Council. Crystallographic development, promotion, and education in Canada are experiencing advances and barriers similar to those seen in the US. The production of high quality data for protein, chemical, material, and scattering analyses is increasing steadily. A set of beamlines for scattering and diffraction experiments at the CLS has been funded. The demand for crystallographic analyses is growing faster than the capacity to train and fund independent crystallographers. As the Canadian representative to Council, I would bring Canadian ideas and perspectives to the table, and encourage Canadian ACA members to become more involved in the operation of our association and the continuing success of our meetings. We are excited about hosting the 2009 meeting, and will make every effort to ensure its success.

Mirek Cygler

Canadian Representative to ACA Council

Principal Research Officer, Biotechnology Research Institute, NRC and Adjunct Professor, Dept of Biochem, and Anatomy and Cell Biology, McGill University, Montreal Canada.

Education: MSc Physics (1970) and PhD Chemistry (1976) Chemistry, University of Lodz, Poland, research associate (1979-1981), Inst. Of Biological Sciences, NRC, Ottawa, professional assistant (1982-1986), Dept. of Biochem, Univ. of Alberta, Edmonton.

Professional Activities: Head, Macromolecular Structure Group, BRI, member of the editorial advisory board of *Protein*

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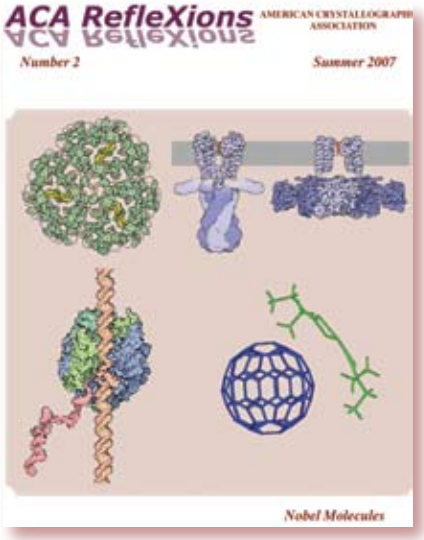
Sci. and the editorial board of *Protein Eng, Des. and Sel*., Co-editor of the 3rd volume of the *Handbook on Metalloproteins*, local chair of the organizing committee of the ACA Meeting (1995) in Montreal, chair of the INPEC steering committee (2002-2003) and organizer of INPEC2002 meeting, organizer of several national and international workshops, *ad hoc* member of the CIHR grant panel, 2004 NRC Outstanding Research Achievement Award, Member of ACA and Protein Society, spokesperson for the X8C beamline, NSLS, BNL, member of the protein crystallography beamline design team, CLS.

Research Interests: Interactions between macromolecules, protein complexes, and enzymatic mechanisms at the molecular level studied by crystallographic and biochemical methods. High-throughput structural biology and automation of all the steps from cloning to structure analysis.

Statement: I have been involved for many years in various aspects of promoting research in the area of crystallography in Canada. The 1995 ACA meeting in Montreal I helped organize was one of the largest and most successful meetings of this association to date. The process of organizing this meeting taught me much about the ACA, its vitality and fellow crystallographers. In the later years I have helped organize the Canadian consortium that has operated the X8C protein crystallography beamline at NSLS, BNL since 1999. This has provided regular access to synchrotron radiation for many Canadian labs, predominantly from eastern Canada. I have also served on the beamline design team that provided advice to CLS staff during the building and commissioning of the first undulator beamline at CLS. More recently, with the substantial growth of the number of structural biology laboratories in Montreal, I have organized the first Structural Biology Workshop in Montreal. The opportunity to represent Canadian Crystallographers at the ACA would be a great honor and would provide me with yet another possibility for contributing to the well being of this exciting multidisciplinary research field in Canada.

What's on the Cover



A quick check of the Nobel website (***nobelprize.org***) revealed at least 20 Nobel prizes have been awarded for research related to structure determination starting with Wilhelm Conrad Rontgen, the 1901 laureate in physics (in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him) through the 2006 chemisty prize to Roger Kornberg. For the cover of this issue of *RefleXions* we have chosen to highlight 4 of these prizes.

2006 (lower left) - ***Roger D. Kornberg*** (Stanford University) for his studies of the molecular basis of eurkaryotic transcription. "Structural basis of transcription: an RNA polymerase II elongation complex at 3.3 Å resolution", A. L. Gnatt, P. Cramer, J. Fu, D. A. Bushnell and R. D. Kornberg, *Science* (2007) **292**, 1876-1882. PDB ID - 1I6H Illustration by David Goodsell (Scripps - ***mgl.scripps.edu/people/goodsell***) from the RSCB PDB (***www.rcsb.org***) Molecule of the Month, April 2003.

2003 (upper right) - ***Roderick MacKinnon*** (Rockefeller University) for structural and mechanistic studies of ion channels. "Chemistry of ion coordination and hydration revealed by a K^+ channel-Fab complex at 2.0 Å resolution", Y. Zhou, J. H. Morais-Cabral, A. Kaufman and R. MacKinnon, *Nature* (2001) **414**, 43-48. PDB ID - 1K4C (right side of figure) and Jiang, A. Lee, J. Chen, M. Cadene, B. T. Chait and R. MacKinnon (2002) *Nature*, **417**, 515-522. PDB ID - 1LNQ (left side of figure). Illustrations by David Goodsell (Scripps) from the RCSB PDB Molecule of the Month, February 2003.

1996 (lower right) - ***Robert F. Curl, Jr***. (Rice), ***Harold W. Kroto*** (University of Sussex) and ***Richard E. Smalley*** (Rice) for their discovery of fullerenes. The illustration shows bis (N,N-diethyldithiocarbamato)-copper(II) C60-fullerene (CCDC REFCODE GAQLUG), one of the more than 600 fullerene structures available in the CSD. D. V. Konarev, A. Y. Kovalevsky, D. v. Lopatin, A. V. Umrikhin, e. I. Yudanova, P. Coppens, R. N. Lyubovskaya and G. Saito, *Dalton Trans*. (2005), 1821. Image drawn using Mercury, version 1.5, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK.

1988 (upper left) - ***Johan Deisenhoffer*** (HHMI - U of Texas Southwestern Medical Center at Dallas), ***Robert Huber*** (Max-Planck Institute for Biochemistry) and ***Hartmut Michel*** (Max-Plank Institute for Biophysics) for the determination of the three-dimensional structure of a photosynthetic reaction center. "Crystallographic refinement at 2.3 Å resolution and refined model of the photosynthetic reaction center from Rhodopseudomonas viridis", J. Deisenhoffer, O. Epp, I. Sinning and H. Michel, *J. Mol. Biol* (1995) **246**, 429-457. PDB ID 1PRC. Illustration by David Goodsell (Scripps) from the RCSB PDB Molecule of the Month, October 2001.

Contributors to this issue of RefleXions

Cele Abad-Zapatero, Jim Britten, Charlie Carter, Mirek Cygler, John Faber, Lee Groat, David Harrison, Chris Hill, Charles Majkrzak, Peter Mueller, Gary Newton, Allen Oliver, Alan Pinkerton, Thomas Proffen, N.S. Rao, John Rose, David Sayre, Harold Shapiro (for photo of Tom Steitz), Eleanor Taylor, Bob Von Dreele, Winnie Wong-Ng

2007 Travel Award Winners

Ernest Asani
New Mexico Highlands University
Bill Bauer
Hauptman Woodward Institute
Julia Bruno Colmenarez
Universidad de Los Andes *Venezuela*
Timothy Colussi
Wake Forest
Janaina Ferreira
Universidade de Sao Paulo *Brazil*
Safiyyah Forbes
Kansas State
Amy Gindhart
University of Toledo
Brett Hanson
Rochester Institute of Technology
Anubhav Jain
Massachusetts Institute of Technology
Christopher Jurgenson
Cornell
Magdalena Korczynska
McGill University *Canada*
Tali Lavy
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Brown University
Jan Lipfert
Stanford University
Xuying Liu
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Bruker AXS, Inc. for sponsoring the Kornberg Lecture

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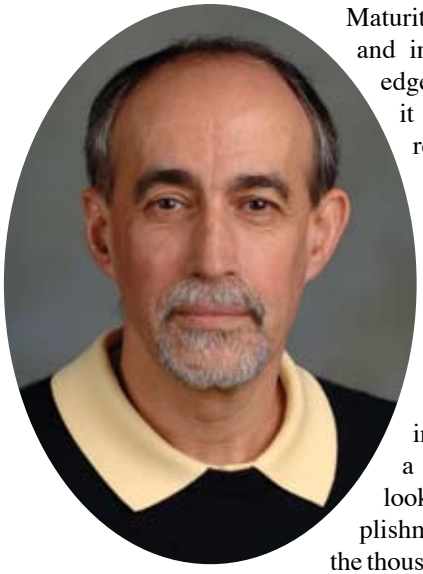
Notes of a Protein Crystallographer: Quo vadis Structural Biology?



Maturity in our personal lives and in science is a double-edged sword. On one side, it is quite satisfactory to reach the middle state in our lives with a sense of accomplishment and pride and look ahead to next stage. Similarly, it is comforting to see the young and revolutionary science that structural biology was in the early sixties reach a point of maturity, and look around at its accomplishments as represented by the thousands of macromolecular structures deposited at the PDB. More important is to examine the critical insights that these structures have provided into in all branches of biology, chemistry, medicine and drug discovery. However, the question is inevitable: What lies ahead? Is it a calm and subdued middle age going to be followed by death, or will there be a rejuvenation and rebirth? Will the future of structural biology lay dormant within the many branches of science that it has helped to advance (biochemistry, cell biology, medicine and others), or will it experience a rebirth by developing new methods to explore the complexity of the living organisms?

This issue has been explored in the last few years by several members of the community. How far and deep we have been able to penetrate into the molecular machinery of biological systems at the beginning of the 21st century, from Vesalius to Palade and Perutz has been insightfully reviewed (Harrison, 2004). After the anatomical discoveries of the renaissance, the structural cell biology tradition of Palade in the first part of the 20th century extended naturally into the structural molecular biology represented by Perutz that we practice today. Harrison's analysis is thoroughly well reasoned and compelling suggesting that the fusion of 'structural molecular biology' and 'structural cell biology' will provide an extended framework for the understanding of biological systems in the next decade. He discusses the roles of structural genomics and computational modeling in that context (Harrison, 2004). This suggested fusion of the two structural traditions represented by Perutz (molecular) and Palade (cellular) will undoubtedly aid in a better understanding of certain biological processes.

The impact of more traditional, well-focused, and slower (i.e. systems-oriented) approaches to discovery in relation to the high-throughput, more expedient (i.e. discovery-oriented), structural genomics strategy was discussed in more detail by Stevens soon thereafter (Stevens, 2004). More recently, Dauter has superbly reviewed the current state and prospects of macromolecular crystallography with a detailed review of the methods and techniques currently in use and the ones that will be appearing in the near future. Both Stevens and Dauter seem confident that the two approaches (high-throughput and specific focus) will continue to provide a constant stream of macromolecular structures that will continue to add to our databases of biological structures and will expand our understanding of living systems (Stevens, 2004; Dauter, 2006). Will this be enough?

I am skeptical that the simple 'structural' extension from molecules to cells will provide the full answers to the complexities of biological systems. A recent essay has been published (Abad-Zapatero, 2007) that provides a historical and scientific context to support this viewpoint. What else do we need? I think that what we need is to the put the living systems within the proper set of physico-chemical principles under which they operate. What is the conceptual framework that encompasses these open, highly heterogeneous and complex systems? The technical term is *dissipative structures*. The term was coined by R. Landauer in 1961 but has been studied, analyzed, and disseminated in the scientific literature by the work of the late Prof. Prigogine (1917-2003) and his coworkers at the Free University of Brussels and the University of Texas at Austin.

In the end, it is the interplay among the conservative molecular entities that we study by single-crystal diffraction methods and the dissipative structures that these molecules make possible that results in the magic of life. This broader conceptual framework suggested above will help us put all this information in the context of systems biology. The concepts of non-equilibrium thermodynamics and dissipative structures have to enter into the domain of modern structural biology if it is to proceed to the next level of understanding. These are concepts that go beyond the commonly accepted notions of intermolecular interactions (be it protein-protein, or protein-nucleic acids) because they include the ideas and notions of flows (fluxes) of matter, energy and information and the sharing of metabolites and chemical intermediates as effectors or facilitators of those interactions. New generations of structural biologists should be introduced to these concepts so that little by little they percolate into the fabric of structural biology and form a part of its intellectual framework. This extension should bring the methods, techniques and *modus operandi* of biochemistry back to the forefront in a novel and more comprehensive way.

Biochemistry is important and I do share the view expressed recently by Arthur Kornberg and others that biochemistry matters "because it does something that genomics, proteomics and other 'omics' cannot yet do" (Kornberg, 2004). As he argues, in the past we have used *in vitro* cell-free systems to gain insights into fermentation, transcription, translation and so many other biological processes. What are those 'cell-free systems' but stable dissipative structures that we can control, manipulate and study their inputs and outputs to infer their complex behavior? We need many more of those self-sustaining systems to gain a deeper understanding of the subtleties of biological systems. This has also been suggested by Harrison (Harrison, 2004) to understand processes ranging from clathrin coating to the motions of the mitotic spindle and beyond. Using the sophistication and experience of traditional biochemists, we need cell-containing or cell-free systems to assay processes such as various biological oscillators,

biological clocks, kinase cascades, cell replication and robust, reproducible and self-sustained signal-transduction systems as well as many other critical biological processes that we do not understand yet at the molecular or cellular level. We may understand the 'parts' but the 'whole' still eludes us.

The use of the concepts and methods of non-equilibrium thermodynamics will aid in understanding the stability, dynamics and control of these open thermodynamic systems and in the design and implementation of new ones. This will open doors to a better understanding of the results obtained by genomics, proteomics and any other 'omics' that we might invent, and will extend to true 'systems biology'. Systems biology modeling should be more than the catalog, description and computer modeling of interactions, no matter how intricate (Giot *et al*., 2003). It should include the detailed spatial and temporal mapping of all components, interacting forces and corresponding fluxes acting on the system. Steven Strogatz, a well known mathematical biophysicist has expressed this idea very concisely: "Our models of complex systems will never advance beyond caricatures until we can find a way to infer local dynamics from data" (Strogatz, 2002).

The insights and understanding gained within this expanded framework will take us from the detailed study of the individual parts at the molecular and pathway level into the true meaning of systems biology, well beyond the simple notion of protein-protein interactions or even protein-nucleic acid interactions (Giot *et al*., 2003). It is conceivable that by expanding our vision of structural biology to include stable, fully integrated dissipative structures, we could open the door to understanding the deregulation existing in the multitude of pathologies associated with cancer, immune disorders, depression and others complex diseases for which our knowledge is still rather limited.

References: Abad-Zapatero, C. (2007). *Acta Cryst*. **D63**, 660-664, Dauter, Z. (2006). *Acta Cryst*. **D62**, 1-11., Giot, L., Bader, J., Brouwer, C., Chaudhuri, A., Kuang, B., Li, Y. et al. (2003). *Science* ***302***, 1727-1736., Harrison, S. (2004). *Nat. Struct. Biol*. **11**, 12-15., Kornberg, A. (2004). *Nat. Struct. Biol*. 11, 493-497, Stevens, R. (2004). *Nat. Struct. Biol*. 11, 293-295, Strogatz, S. Fermi's "Little Discovery" and the Future of Chaos and Complexity Theory. In *The Next Fifty Years. Science in the First Half of the Twenty-First Century.* p. 121. Edited by John Brockman. Vintage Books. A Division of Random House Inc. New York. 2002.

Cele Abad-Zapatero

"Molecular anatomy will be the foundation of medicine in the 21st century , as was human anatomy five centuries earlier […]. In as much as synchrotron radiation is the primary means by which large scale biological structure information will be obtained in the future, continued support is of utmost importance"

Arthur Kornberg

John W. Backus- Father of Fortran - (1915-2007)

In March a note posted to the CCP4 news group stated that John W. Backus, the 'father of Fortran', had passed away.Backus assembled and led the IBM team that created Fortran (short for Formula Translator) which was first released in 1957. The NY Times obituary (March19, 2007) stated that Mr. Backus and his youthful team, then all in their 20s and 30s, devised a programming language that resembled a combination of English shorthand and algebra. It was very similar to the algebraic formulas that scientists and engineers used in their daily work. With Fortran they were no longer dependent on a programming priesthood to translate their science and engineering problems into a language a computer would understand. His team was an eclectic bunch that included a *crystallographer*, a cryptographer, a chess wizard, an employee on loan from United Aircraft, a researcher from the Massachusetts Institute of Technology and a young woman who joined the project straight out of Vassar.

* *

A second note posted to the news group by Bob Sweet included the following: I'm pretty sure that the crystallographer was David Sayre, known in crystallography for the Sayre's Equation (*Acta Cryst*. 5, 60-65 (1952) a fundamental relationship in direct methods. Also, maybe not so well known, he has been a major driving force behind the method of visualizing single molecules or cells from diffraction patterns: (J. Miao, H. N. Chapman, J. Kirz, D. Sayre and K. O. Hodgson, Taking X-ray Diffraction to the Limit: Macromolecular Structures from Femtosecond X-ray Pulses and Diffraction Microscopy of Cells with Synchrotron Radiation, *Ann. Rev. Biophys. Biomol. Struct*. **33**, 157-176 (2004).)

He and I used to use adjacent darkrooms at the NSLS for developing x-ray films (the '80's). I'd meet him on the long walk, ask what he was doing, and smile sympathetically when he said he was going to image single yeast cells. Well, they're essentially doing it now. One never wants to underestimate David Sayre's ability to find phases.

(Editors note: David spoke on this project at the IUCR Congress in Florence where he described the technique used in the 2D imaging of the yeast cell (Acta. Cryst **A62***, 248-261 (2006) and he is now working on extending this to 3D imaging).*

* *

To test Bob Sweet's memory the editor followed up with a note to David asking if he really was that crystallographer and was extremely pleased to receive the following:

In 1954 Peter Friedlander and I were at the Johnson Foundation of the University of Pennsylvania, working on the structures of benzanthracene and 7,12-dimethylbenzanthracene (7,12-DMBA), hoping to cast some light on 7,12-DMBA being a much stronger carcinogen than benzanthracene itself. Peter, working on benzanthracene, was finding a planar polycyclic structure, but 7,12-DMBA, which at that time was generally thought of by chemists as also being planar, was showing signs of crowding of the methyl groups and non-planarity. Wishing to check further, we decided to see whether least-squares 3D refinement would confirm this difference in the structures. At that time the only 3D least-squares program was Durward Cruickshank's program for the MADAM computer in Manchester England, but there was a closer machine, an IBM

701 at IBM's corporate headquarters in New York City, and IBM kindly offered a little time on the machine for the project. I wrote the program, and the non-planarity of 7,12-DMBA, as well as the planarity of benzanthracene, was confirmed. (I discover now, in the modern literature on carcinogenicity, that the structure of 7,12-DMBA enables it to attach strongly to DNA, so that we had indeed in 1954 stumbled on at least some of the reason for its carcinogenicity.)

The reader might be interested to know how the programming was done in 1954. There was an assembly program for the 701, but sitting in Philadelphia I was unable to make much sense of it, and I ended by writing the program in absolute octal. In addition, the storage-tube memory of the 701 was not very reliable, so the practice was to have each major stretch of code in the program occur twice, and not proceed if the two answers did not agree. Warner Love was with me when we took the hand-punched deck of 0's and 1's to New York to try it, and it got stuck. That night one of us read the octal version aloud to the other, who was following on the cards. We found one mis-punched bit, and the next morning, when we corrected that, the program ran.

I very much enjoyed the whole experience, so when I was asked if I would like to stay on with IBM I accepted, and early in 1955 found myself in a group which was writing software for the IBM 704, that was going to be the successor to the 701. Quite near to us was John Backus's group, working on Fortran for the 704. John, Harlan Herrick, Peter Sheridan, and Irving Ziller had worked out the main features of the Fortran language, and had taken it to the 701 users, who said that they liked it, but doubted if the Fortran processor would be able to produce really efficient programs from it. John and the others took this as a challenge, and started work. At some point in 1956 John asked to borrow me to help deal with a situation which had developed. The opening Section 1 of Fortran (arithmetic statements; Harlan Herrick and Peter Sheridan) was nearing readiness, as were Section 2 (DO statements; Irving Ziller and Bob Nelson) and Section 3 (most remaining statements other than input/output; Dick Goldberg). Section 2, however, treated the DO statements as if the 704 came equipped with an unlimited number of index registers, whereas in reality it had only 3. John had borrowed Sheldon Best, a brilliant young programmer at MIT, to deal with that problem, and Sheldon had devised a brilliant Section 4 and Section 5 to do it. Lois Mitchell Haibt was programming Section 4, and Sheldon was partway through the programming of Section 5. At this point, however, his leave from MIT was ending. John therefore put together a new team (Dick Goldberg and myself) to finish Section 5, and we had it working by the spring of 1957. Roy Nutt, an outstanding programmer from United Aircraft in Hartford, then wrote Section 6 (input/output), and in 1957 the system was distributed, and was an immediate success. From the start it was noted for the efficiency of the programs which it created.

The Fortran group was the happiest work-group I have ever known. John Backus provided cheerful and highly intelligent leadership, and was always thoughtful of other people. Everyone engaged in the project loved it and believed in the importance of what they were doing. It has been a pleasure to re-live it now.

David Sayre

Fourth Annual SER-CAT Symposium, National Cancer Institute, Frederick, MD

"Interesting Structures, Methods and Advances in SER-CAT Facilities," was the theme of the 2007 Annual SER-CAT Symposium, which was held on March 16, 2007 in Frederick, Maryland, and hosted by ***Alex Wlodawer*** at the National Cancer Institute. Approximately 70 people were in attendance. As in 2006, practical aspects of tools and improvements made at the SER-CAT beamlines, from a user's perspective, were highlighted. The meeting served as an informative and interesting forum where users share their recent significant crystallographic research discoveries. Also, attendees were delighted with the bonus of a late snow storm, giving extra excitement to the meeting's activities.

The morning session opened with the presentation of the first SER-CAT Golden Magnolia Award to SER-CAT Director ***Bi-Cheng (B.C.) Wang*** for his distinguished service to SER-CAT. B.C. was recognized by the SER-CAT Executive Board and colleagues for his ten years of dedicated service and conscientious guidance of the program from inception to SER-CAT's current status as one of the most productive beamlines in the nation. After a brief ceremony where ***John Rose*** (SER-CAT Assistant Director) presented the Golden Magnolia award, B.C. told about the history of the development of SER-CAT from 1997 to present: "SER-CAT: The First Ten Years." B.C.'s talk (PDF format) can be found on the SER-CAT website ***www.ser-cat.org.***

The morning session, chaired by ***Xinjua Ji*** (NCI at Frederick), consisted of eight talks under the general subject of "Interesting Structures". The invited speakers and their presentations were:

Christopher Davies (Medical University of South Carolina) "Structural changes in gonococcal penicillin-binding protein 2 associated with antibiotic resistance." He described his work toward understanding the biological function of these proteins in hopes of targeting them for therapeutic intervention.

Irene Weber (Georgia State) "Targeting HIV-1 drug resistance: Darunavir complex with V32I mutant of HIV protease at 0.84 Å resolution." She discussed her research on anti-AIDS therapies and the molecular basis of drug resistance. In her work, she hopes to improve the effectiveness of drugs against multi-drug resistant variants.

Yong-Fu Li (NIH, National Cancer Institute) "Biogenesis of CFA/I fimbriae of enterotoxigenic *E. coli*." He described how he utilized a solved crystal structure to help understand a common, but bothersome ailment: diarrhea. In his work he hopes to understand the mechanism of binding and provide preventative treatments for the sickness.

David Garboczi (NIH, NIAID-LIG) "Structural analysis of surface proteins of the malaria parasite." He discussed how malaria parasites invade the tissues of hosts and specific cell-types. His research is geared toward designing drugs for anti-malaria vaccines and gaining better understanding of the biology of the malarial parasite as a whole.

Robert Rose (North Carolina State) "Small angle scattering as an approach to model a multi-protein complex on the insulin promoter." His work in diabetes research showing how insulin reacts to beta cells should ultimately aid in diabetes drug therapies.

Jacek Lubkowski (NCI Frederick) "CCR-mediated chemotaxis of human B-defensins: structural basis" as it pertains to chemotaxis proteins and viral infections. His work is geared towards the treatment of immune disorders and improved drug therapies.

Before the afternoon lunch hour, acknowledgements for both the 2007 SER-CAT Young Investigator and Outstanding Science Awards were presented. For the third year, SER-CAT took the opportunity to recognize the outstanding achievements made by individuals at the SER-CAT facility.

Each year the young investigator award is presented to an individual who is at least two years away from their PhD and has displayed an important technical or scientific accomplishment at, or of benefit to SER-CAT. For 2007, ***Ping Liu*** (Georgia State) received this Award for her work on the "Crystal structure of the *Geobacillus stearothermophilus* carboxylesterase Est55 and its activation of prodrug CPT-11," which has been published in the *Journal of Molecular Biology*.

The SER-CAT Outstanding Science Award is given to a researcher or research group carrying out important and beneficial experimental work at SER-CAT. This year, ***Michael Wiener*** (University of Virginia) received the award for his paper entitled, "Outer membrane active transport: Structure of the BtuB:TonB complex," because it proved to have the highest scientific impact out of all papers received. Both awardees gave a 20-minute talk on their recognized works at the symposium.

After lunch, a poster session and remote access demonstration were provided, followed by a plenary lecture by ***Cynthia Wolberger*** (Johns Hopkins) entitled "Mechanisms of lysine modification: The Sir2 Deacetylase and Lys63-linked Polyubiquitin Chain Assembly." She presented an insightful presentation on proteins in cellular function and gene expression.

The afternoon session, chaired by ***David Waugh*** (NCI at Frederick), consisted of five talks under the general subject of "Methods and Advances in SER-CAT Facilities." The invited speakers and their presentations were:

Jiawei Wang (NCI, Argonne National Lab) "Statistical Distribution of Bijvoet differences," a discussion of the varying distribution of Bijvoet ratios in structural crystallography research for improved results.

Wladek Minor (University of Virginia) "HKL-3000 – Towards the Future of Protein Crystallography." Wladek gave an interesting demonstration of the HKL-3000 capability in solving protein structures.

Denny Mills (Argonne National Lab) "The Advanced Photon Source - Now and in the Future," highlighted the accomplishments and future goals of the APS facility.

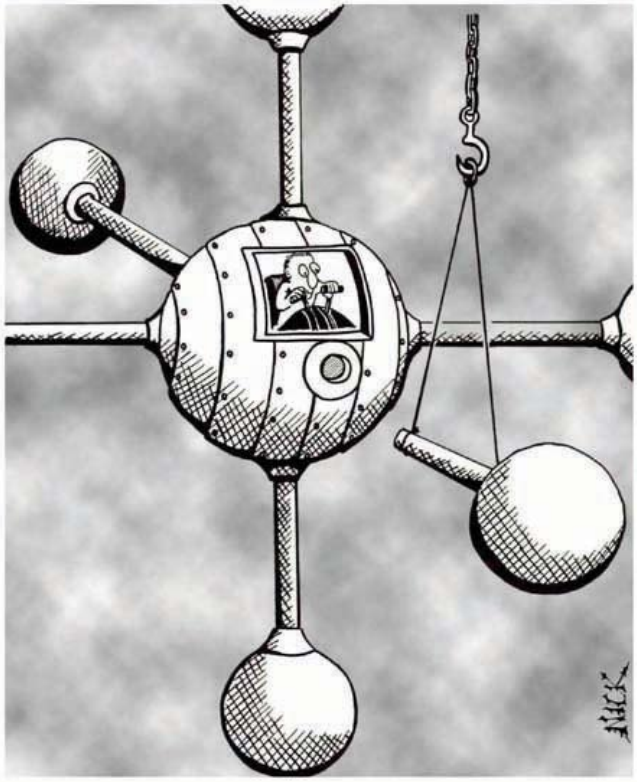
John Chrzas (UGA/SER-CAT)"The SER-CAT Virtual Home Facility," about the possibility of taking home SER-CAT results in a virtual capacity.

Zheng-Qing (Albert) Fu (UGA/SER-CAT) "The SER-CAT on-site Data-to-Structure Capability," about the advances at SER-CAT allowing users to quickly obtain the structural models of the data collected while still at SER-CAT.

The meeting closed late in the afternoon with more conversations and shared experiences. The day was filled with insight, expertise and a wealth of information for those who attended. The meeting served as another opportunity to learn techniques and new innovations in the field of crystallographic research in relation to health and technology. We would like to thank all of our attendees, as well as our host Alex Wlodawer and his staff for their hospitality and assistance in making this year's meeting a success. If you would like additional information on this year's event, including more photos, please visit us online at ***www.ser-cat.org***.b

The site for the 2008 Fifth Annual SER-CAT Symposium will be announced soon; check the SER-CAT web site for details.

Gary Newton



The mysterious world of ligand substitution (by Nick D. Kim, U. Waikato, NZ - nearingzero.net/res.html)

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2006 and 2005

	CURRENT FUNDS (2006)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2006	2005
ASSETS				
Current Assets:				
Cash	251,432		251,432	175,550
Investments	316,742	362,704	679,446	790,478
Inventory	5,600		5,600	5,600
Total Current Assets	573,774	362,704	936,478	971,628
Fixed Assets:				
Computers and Printers	4,598		4,598	4,598
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	5,898		5,898	5,898
TOTAL ASSETS	579,672	362,704	942,376	977,526
Liabilities:				
Deferred Dues Income	14,138		14,138	0
Total Liabilities	14,138		14,138	0
Fund Balance:				
Unrestricted	565,534		565,534	624,611
Restricted		362,704	362,704	352,915
Total Fund Balance	565,534	362,704	928,238	977,526
TOTAL LIABILITIES & FUND BALANCE	579,672	362,704	942,376	977,526

*** Current Balances in individual restricted funds - as of December 31, 2006**

Buerger Award	35,887
Etter Award	64,083
Fankuchen Award	67,530
Patterson Award	40,328
Pauling Award	32,187
Supper Award	10,616
Trueblood Award	32,659
Warren Award	29,148
Wood Science Writing Award	50,266

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY

Calendar of Future Meetings

JULY 2007

1-6 **Gordon Research Conf. on Electron Distribution and Chemical Bonding,** Mt. Holyoke Coll., MA

9-18 **ACA Summer School in Small Molecule Crystallography**, Indiana University of PA, **craven@icubed.com** or **lake@iup.edu.**

21-26 **ACA - Salt Lake City, Utah.** *Local Chairs: Chris Hill (Utah, chris@biochem.utah.edu) & Heidi Schubert (Utah, heidi@biochem.utah.edu), Program Chair: Jill Trewhella (Univ. of Sydney), b2jtrewhella@usyd.edu.au.*

29-8 **Small-Molecule Crystallography Summer School,** San Diego, CA. Arnold L. Rheingold, **arheingold@ucsd.edu; http://chem-tech.ucsd.edu/Recharges/SMXF/crystalschool.html.**

AUGUST 2007

13-17 **BSR2007: 9th International Conference on Biology and Synchrotron Radiation,** Manchester, UK. **www.srs.ac.uk/bsr2007/.**

22-27 **ECM-24** Marrakech, Morroco. **www.ecm24.org.**

SEPTEMBER 2007

3-6 **Advanced Methods in X-Ray Charge Density Analysis,** Martina Franca, Italy. **piero.macchi@unimi.it, nicola.casati@istm.cnr.it, simona.galli@uninsubria.it.**

NOVEMBER 2007

4-7 **AsCA - Asian Crystallographic Association Meeting, Taipei,** Taiwan R.O.C. **www.asca2007.tw/index.html.**

MAY 2008

29-June 8 **From Molecules to Medicine, Integrating Crystallography in Drug Discovery** Erice, Italy.**www.crystalerice.org/erice2008/2008.htm.**

31-June 5 **ACA Annual Meeting -Knoxville, TN** *Local Chair: Jason Hodges (SNS Division - ORNL, hodges@ornl.gov). Program Chair: Paul Butler (NIST,* **butler@nist.gov***).*

AUGUST 2008

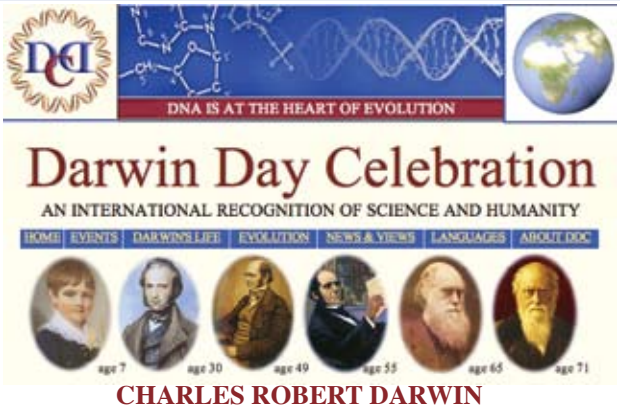
21-28 **IUCr2008:** 21st Congress of the International Union of Crystallography, Osaka, Japan. **congre.co.jp/iucr2008.**

JUNE 2009

4-14 **High Pressure Crystallography: From Novel Experimental Approaches to Applications to Cutting Edge:** Erice, Italy. **www.crystalerice.org/2009.htm.**

JULY 2009

25-30 **ACA Annual Meeting - Toronto - Ontario - Canada** *Program Chair: Jim Britten (McMaster University, britten@mcmaster.ca).*



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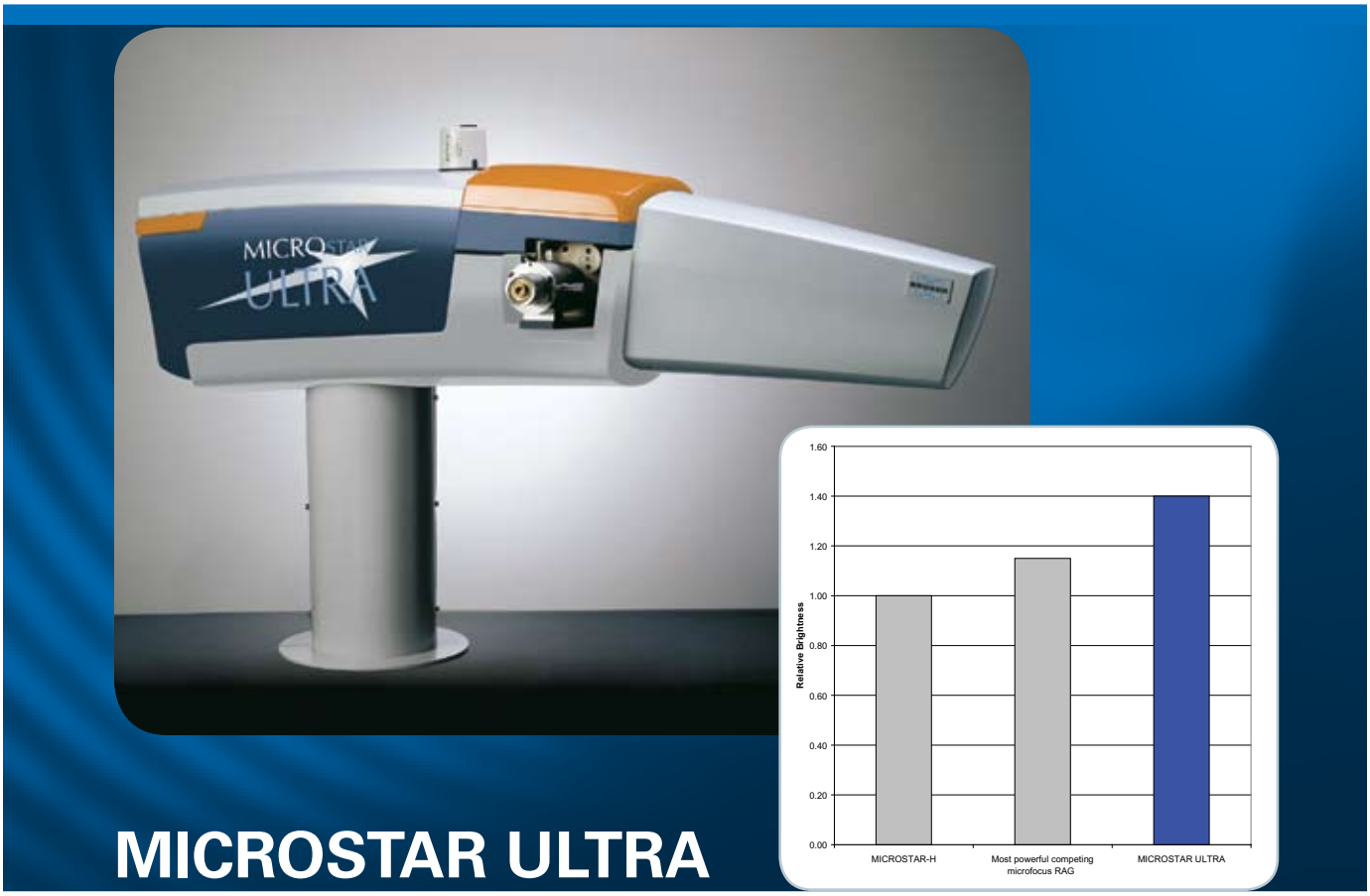

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Quite simply: What matters most is the diffracted intensity from your sample. The MICROSTAR ULTRA is the brightest laboratory X-ray source available. The ULTRA boasts a brightness 25% higher than the next closest competitor. This means that on your real world samples, you see more diffracted intensity and better signal-to-noise.

But don't just take our word for it. Put your crystals on the MICROSTAR ULTRA and see for yourself!

Contact us for more details and system demonstration! **www.bruker-axs.com**

think forward

Crystallography