

5th Annual CLS Users' Meeting and Workshops - November 15-17, 2002

Summary

The fifth annual CLS users' meeting was held at the University of Saskatchewan on Nov 16 with four associated workshops being held on Nov 15, 2002. It was a resounding success. Over 300 people registered for the workshops and / or the users' meeting. The meeting was organized by the 2002 CLS Users' Advisory Committee (UAC), and chaired by *Stephen Urquhart* (U. of S.), chair of the UAC. The highlight of the meeting was the welcoming to the community of our new executive director, *Bill Thomlinson*, who gave a rousing and impassioned presentation, which will be remembered as a defining moment in the history of CLS. This document summarizes the activities and provides a photo record of the events.

Workshops – Friday Nov 15

Four workshops were held.

The **Materials Science workshop** was organized by *Karen Kavanagh* (SFU). The morning session consisted of overview presentations about the materials research programs at four of the US national synchrotron facilities. *Murray Gibson* (APS) outlined the many exciting programs in hard x-ray science at the APS. *Neville Smith* (ALS) indicated the special role ALS plays among the four DoE facilities in providing world leadership in soft x-ray techniques. He noted that the recent adoption by the semiconductor industry of extreme ultraviolet lithography as the preferred lithographic technology for sub-70 nm scale devices (post 2004) was directly a consequence of the extensive program on optics and systems testing that Intel and others have carried out at the ALS over the past 3 years. This work alone justifies both the capital and operating costs of the ALS. *Franz Himpsel* (SRC) described the strong programs in angle resolved photoemission, microscopy and nanotechnology at SRC. *Steve Dierker* (NSLS) outlined the very broad and sustained programs in materials science at both of the rings at NSLS. In the afternoon, *Pat Mooney* (IBM) outlined how research using diffraction techniques at the NSLS and APS was providing key information for optimization of technologies key to IBM's advanced Si technologies. Capabilities for tracking electro-migration in real time as well as extensive analytical matrix approaches to solving materials problems were described. *Tony van Buuren* (LLNL) described his groups' use of X-ray absorption spectroscopy to study novel nano-scale systems such as quantum dots and molecular switches. *Carol Thompson* (Northern Illinois U) presented her groups' work at the ALS on *in situ* studies of materials growth by metal-organic chemical vapour deposition. The last presentation of the workshop was



Bill Thomlinson listening intently in the Materials Science workshop.



The ALS is the only third generation dedicated soft X-ray source in the US.

given by *Andrea Damascelli* (UBC) on angle-resolved photoemission studies at SSRL, which probe the mechanisms of high temperature superconductivity. The recent advances in machine brightness and electron spectroscopy have together provided an overall energy resolution in the few meV range which is revealing direct information about the coupling mechanism(s) involved. Over 50 people were in attendance at all times during the day and over 70 people registered. Judging by the excellent presentations, the extensive questioning, and active hallway discussions, this session was very successful at informing the CLS community about the wide variety of applications of synchrotron research to materials science.

The **Environmental and Industrial Science** workshop was organized by *Jeff Cutler* (CLSI) and *Brett Moldovan* (Cameco). Its goal was to present attendees with highlights of synchrotron applications to environmental science, particularly those relevant to the mining industry, along with other industrial applications. The workshop began with a presentation by *Mike Bancroft* (UWO) on the industrial program of CLSI. *Masoud Kasrai* (UWO) then described his use of soft X-ray spectroscopy and microscopy to develop fundamental understanding of combustion engine tribological coatings, both existing and potential replacements. *Irina Snigireva* (ESRF) outlined environmental applications of hard X-ray microprobe and microdiffraction techniques. Of particular interest to the attendees was a study using microtomography techniques to characterize radioactive fuel particles released from the Chernobyl reactor. *Ken Reimer* (RMC) finished the morning session with a presentation on potential uses of synchrotron light to study arsenic speciation and possible bio-availability in the environment. The afternoon session began with a description by *Neil Sturchio* (U. Illinois Chicago) on studies of mineral water interfaces with X-ray reflectivity techniques. This interface is of critical importance to many environmental problems. *Frank Huggins* (U. Kentucky) showed how X-ray absorption fine structure and other synchrotron methods were being used to characterize sulphur and various heavy metals in airborne combustion particulates less than 2.5 microns in size (PM_{2.5}). *Trevor Bergfeldt* (Teck Cominco) outlined the use of X-ray absorption to characterize arsenical materials from a Teck Cominco mining site in BC. Particularly, x-ray absorption results were presented that demonstrated that a baghouse dust that was previously characterized as amorphous by x-ray diffraction techniques was actually very crystalline. The last two presentations were focused on procedures to deliver value-added synchrotron research to industrial clients. *Robert Audette* described ISO/IEC 17025 laboratory accreditation methodologies and potential synchrotron applications. This talk led to some good discussions on the challenges that a synchrotron facility would face in meeting the requirements of the laboratory accreditation program. Many of the people in the audience felt that the essence of synchrotron science is that it is “cutting edge” and therefore a well-defined set of procedures and QA programs that are the basis of the accreditation policies would be difficult to maintain. *Elizabeth Maclean* (Daresbury) closed the workshop out with a description of the fee-for-service program at Daresbury along with a series of interesting examples associated with delivering synchrotron science to industrial users.

The **Biological / Life Sciences** workshop was organized by *Gerald Audette* (U. Alberta). It was aimed at highlighting recent advances in the life sciences derived from synchrotron radiation research. The session began with a thorough presentation by *Chris Jacobsen* (SUNY-Stony Brook) on uses of soft X-ray scanning transmission X-ray microscopy for studies of biological and environmental samples in the wet, frozen state at 30 nm spatial resolution. In addition to illustrating the power of this technique, Chris outlined recent advances in phase contrast, dark-field imaging, and direct space methods of structure determination of irregular objects using coherent soft X-rays. *Tom Irving* (APS)

introduced the audience to the BioCAT facility at the APS, designed for the examination of non-crystalline biological systems using small-angle scattering. Tom detailed recent studies into muscle contraction, and the lengths that one must go through to obtain time-resolved data on muscle contraction from live, immobilized fruit flies. *Ke Zhang* (APS) outlined recent instrumentation developments at the APS to enhance extended X-ray absorption fine structure measurements of dilute biological systems. Advancements in energy selective multi-layer detectors coupled with high count-rate photomultiplier tubes (PMTs) and sample flow-cells are enabling time-resolved XAFS studies on more dilute samples while improving spatial resolution and signal-to-noise ratios. *Steve Wilkins* (CSIRO) introduced the audience to the Australian synchrotron project located at Monash U. in Melbourne, aptly nick-named “Boomerang”. Steve also introduced the audience to phase contrast imaging and phase/amplitude retrieval techniques in hard X-ray diffraction. The aim is obtaining quantitative information through X-ray imaging for diagnostic purposes, and Steve showed some impressive results from some recent soft tissue studies.



An attentive audience at the life sciences workshop.

After lunch, *Zbigniew Dauter* (NSLS) provided a tutorial on recent developments in single-wavelength anomalous dispersion (SAD) phasing for protein crystallography, with emphasis on the use of quick halide soaks for introduction of the anomalous signal. It seems we may not need to go MAD to solve crystal structures!! *Ashley Deacon* (SSRL) outlined the SSRL structural genomics program investigating the genome of *Thermatoga maritima* using high throughput protein crystallographic techniques. Ashley highlighted the advances in beamline automation required in order to undertake such a project, including automated crystal mounting, centring and diffraction analysis; he also provided a glimpse into the wealth of structural information that can be obtained, including the identification of several novel protein folds not observed before. *Bernhard Juurlink* (U Saskatchewan) concluded the workshop with a description of his experiences as a new synchrotron user. Bernhard began with the question “What can the synchrotron do for me and my research?”, and he highlighted a number of recent studies from the emerging biomedical synchrotron group at U of S. Together with *Kathy Gough* (U Manitoba), Bernhard’s group have begun mapping macrophage infiltration to sites of injury through lipid identification using infrared spectroscopy, and are examining the effects of anti-oxidants to reduce scarring of spinal tissue following surgery. The workshop was well attended, and the excellent presentations, numerous questions and lively conversations during the breaks all contributed to the success of the session.

The **High heat load and Novel X-ray Optics** workshop was organized by *Emil Hallin* (CLSI) and held in the afternoon. It opened with a description by *Anatoly Snigirev* (ESRF) of exciting new developments in hard X-ray microfocusing. *Deming Shu* (APS) then gave a tutorial on issues relating to design of front-end components in high heat load conditions. *De-Tong Jiang* (CLSI) then outlined the optical design of the micro-XAFS beamline at the CLS. Recent evolution of this design has reached the point where it is a fully competitive hard X-ray microprobe facility, in addition to providing high flux spectroscopy. *Ian Coulthard* (CLSI) then described the optical design of the intermediate energy

microprobe, an evolution of the tender X-ray double crystal monochromator originally envisaged for CLS. The last formal presentation by Brian Yates (CLSI) was a description of the CLS optics metrology lab. The workshop ended with a round table discussion on various X-ray optics issues.

Users' Meeting – Saturday, Nov 16

The meeting was opened by *Stephen Urquhart*, chair of the CLS Users' Advisory Committee and of the meeting. After welcome and organizational comments. *Bill Thomlinson*, the newly installed executive director, gave some words of welcome and introduced himself to the CLS community. *Mark de Jong*, the project leader of CLS, then outlined the status of the project, both accelerators and beamlines. The booster ring commissioning went significantly faster than planned so that full specifications were achieved and the device formally accepted from Danfysik in Sep-02. The storage ring parts are either at CLS or arriving daily. Much of the support structure has been installed and magnet and vacuum tank installation will be carried out before the end of the year. It is anticipated that storage ring commissioning will begin in March of next year, with anticipated periods of operation suitable for beamline commissioning activity becoming available in the fall of 2003. Overall the project is on time and on budget, although a few of the beamlines – protein crystallography and the hard X-ray spectroscopy / microprobe lines might be delayed into early in 2004. Following this report, *Les Dallin*, head of the accelerator group at CLS, gave a detailed report on the booster ring commissioning.

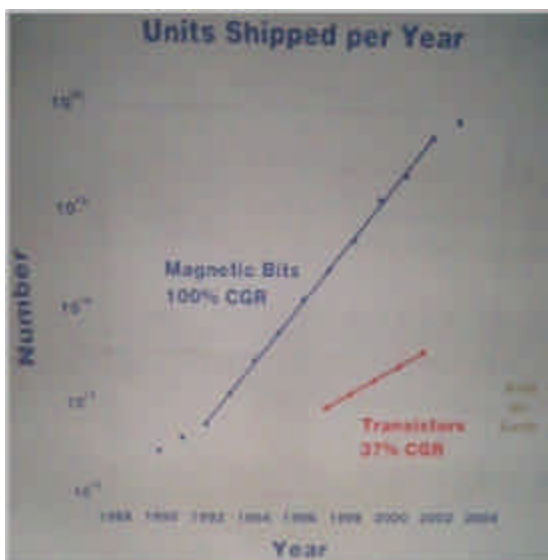
The scientific highlights program of the users' meeting began with a presentation by *Glenn Waychunas* (Earth Sciences, LBNL) on X-ray absorption spectroscopy applied to environmental science. He stressed the complexity of these systems and the need to study processes relevant to many different time and spatial scales in order to properly understand and hopefully control environmental contamination issues. *Larry Sorensen* (U. Washington) gave a lucid presentation of the emerging technique of soft X-ray speckle and its use to study dynamics of magnetization. This technique exploits both the coherence and tenability of third generation undulator radiation from the ALS to



Stephen Urquhart opening the 5th CLS Annual Users' Meeting

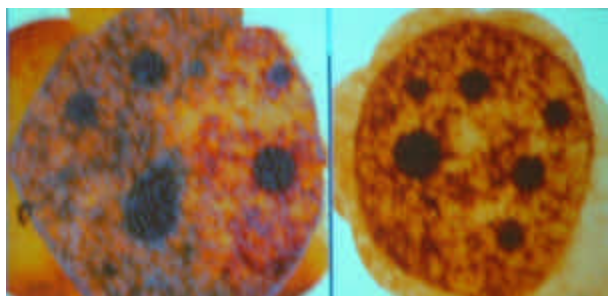


Booster ring in operation



Larry Sorensen explaining the impact of speckle studies of the dynamics of magnetism to the data storage industry.

measure speckle patterns of magnetic materials.



X-ray micrograph locating pores leading into a cell nucleus. Highlighted by protein specific Au/Ag labels, present in the left image and absent in the control (right). (C. Larabell, UCSF, ALS)

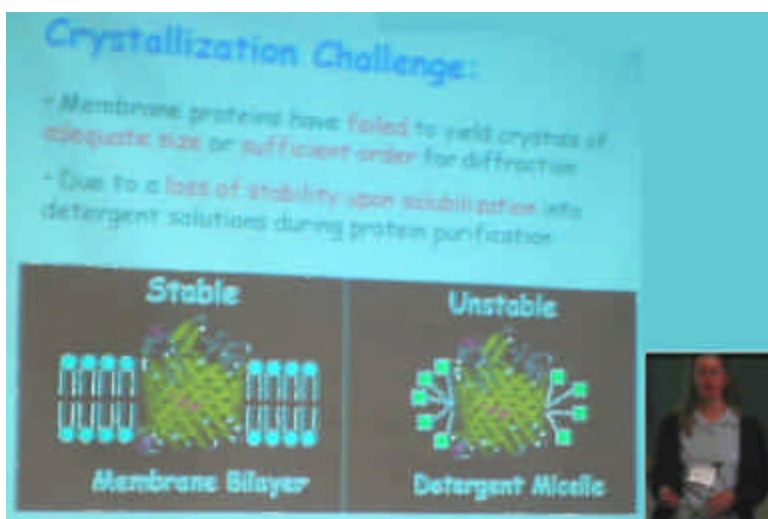
The last three presentations of the morning session highlighted the research programs of new Canadian faculty members or researchers.

Michelle Loewen (PBI, UoS) described her program to develop methods to crystallize membrane proteins and solve their structure. Although such proteins dominate the genome and are the targets for most pharmaceuticals, very few structures have been solved to date because of the great difficulty to form suitable crystals. *Andrea Damascelli* (UBC) described in a highly tutorial fashion the role of synchrotron based high-energy resolution angle resolved

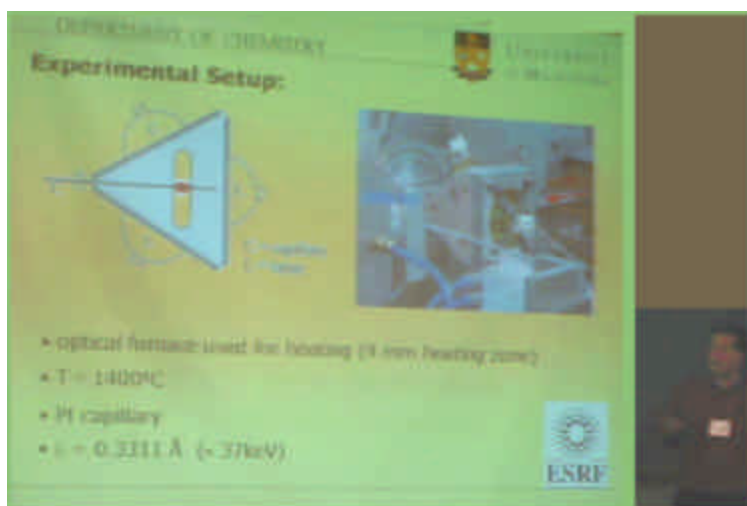
photoemission is playing in correlated electronic materials such as the high critical temperature superconductors.

Mario Bieringer (Manitoba) described his studies with synchrotron powder diffraction to measure the chemical structure of piezoelectric materials critical to wireless technology. The technology to carry out in situ structure studies at 1400 C was very impressive.

Carolyn Larabell (UCSF, ALS) gave perhaps the most visually compelling presentation of the meeting, with a spellbinding presentation on correlated use of confocal optical, soft X-ray full field transmission, and electron microscopies to study detailed biochemical pathways at the sub-cellular level. Time-lapse photography with genetically introduced fluorescent labels, soft X-ray microscopy of well cells, and computer-aided microtomography for 3-d views of yeast cells were all illustrated.



Advanced crystallization methods are being developed and applied to membrane proteins by Michelle Loewen (PBI, UoS)



Mario Bieringer described novel high temperature powder diffraction experiments for probing structural changes in piezoelectric materials critical for wireless applications.

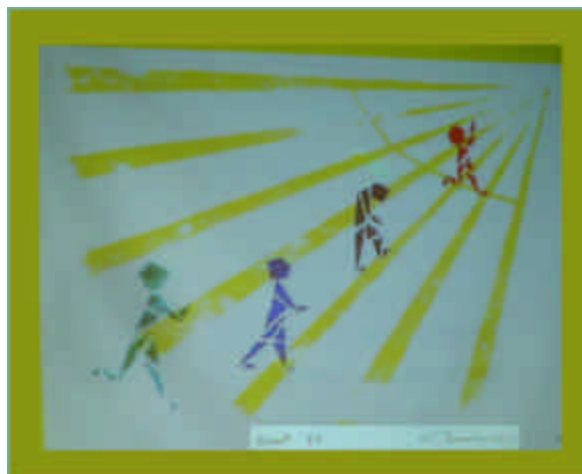
During the lunch break three breakout sessions were held, in which CLS community could provide feedback to CLS management on issues of concern. Brief reports from each of these sessions are included below.

- * User Access (*Tom Ellis*, facilitator) ~ 15 attended
- * Growing the CLS User community (*Gerald Audette, Nancy Bernini*, facilitators) ~ 15 attended
- * Phase II beamline procedures (*Tom Tiedje*, facilitator) ~ 30 attended

The afternoon began with a session on industrial use of synchrotron radiation. *Gary Mitchell* (Dow chemical) presented some of his recent work on trouble shooting and product development research at Dow. He emphasized how the unique chemical sensitivity at high spatial resolution of scanning transmission X-ray microscopy was uniquely able to solve some problems of high economic importance to Dow. In the last part of his presentation Gary showed how modern industrial research is driven not just to use advanced synchrotron techniques, but also to invent new ones. In particular he described how he and his colleagues have developed the first use of resonant soft X-ray scattering to provide chemically sensitive structural characterization of polymers at the 5-20 nm spatial scale. This regime is essential to developing nanostructure aspects of the SiLK™ technology of spin-on low dielectric insulator that Dow is currently marketing to Silicon Valley for next generation processing. The one-year time frame from concept to demonstration, to application of the new technique was driven by the ‘pre-programmed’ development schedule of the semiconductor industry. The last presentation of the scientific program was by *Michael Hagelstein* (ANKA) who described the program and beamlines for industrially-oriented service research of the Karlsruhe ANKA facility. A major component is support for the LIGA micro-mechanical technology that was first developed at Karlsruhe.

The mid-afternoon session was used to carry out the business of the CLS Users’ Advisory Committee. *Stephen Urquhart* (U. of S.) described the activities of the UAC over the past year. This was followed by reports from the facilitators on the three breakout sessions (see below). Nominations for replacement members of the UAC were then held, resulting in a large number of nominations from the floor. As a democratic organization, the UAC is flourishing. The election of new members will begin on Dec-09 via the web.

After an extended coffee break, which featured animated discussion with vendors, and poster presenters, the President of the University of Saskatchewan, *Peter MacKinnon* made extended comments on the relationship of CLS and the U. of S. He then introduced *William Thomlinson*, Executive Director, CLS as of 1-Nov-02. In a well crafted, humorous, passionate, and informative presentation, Bill outlined his vision for the CLS. In it he stressed his number one priorities of improving communication, developing user-oriented programs and procedures, expanding as rapidly as possible the scientific capabilities of CLS through new beamlines, and ongoing vigilance on safety. He concluded with a very personal note based on his experience as a marathon runner. After a jubilant start, the runner settles into a steady pace. Towards the end, invariably



Bill Thomlinson, Quest, New York marathon, 1977.

there is ‘the wall’ - that black period well into a race in which the runner is exhausted and may doubt their ability to complete the course. Bill noted that, although CLS is currently in that phase, it is also close to the finish line – which in a marathon is traditionally also the START line. He encouraged the CLS staff and community to ‘hang in’ and to look forward, after a further 12-16 months of hard work, to arriving at the start of a new and invigorating phase, that of operations. His exceptional, very personal, presentation was recognized with a standing ovation.

Following the oral presentations of the meeting, there was a 2-hour poster session in the Geology Atrium, where the attendees were able to view and discuss over 50 posters. Simultaneously, tours of the CLS were carried out.

The meeting banquet was held in Marquis Hall. After dinner the CISR travel award was presented to *Gianfranco Mazzanti*, a postdoctoral fellow with *Stephan Idziak* at Waterloo University. This \$1000 award will be used to support travel by the winner to a conference in 2003.

Beamline Team meetings – Nov 17

During Sunday meetings were held by each of the phase I beamline teams, and by the phase II beamlines in the phase of conceptual design and fund raising.

APPENDIX: Breakout session reports

The following is a summary of comments and discussion at the lunchtime breakout sessions.

User Access (*Tom Ellis*, facilitator) ~ 15 attended

The breakout session on user access issues was attended by about 15 people, most of whom were not members of beamteams.

To start the meeting, Tom Ellis explained the process whereby Beamline Agreements would be negotiated between the Beamteams and the CLS. It was emphasized that these Agreements would determine the amount of beamtime that was available to each type of user. Those who are not members of Beamteams are not directly represented in these negotiations, although their interests are being considered by all parties. The UAC should make it a priority to represent “general users” during the negotiations.

There was a clear acceptance of the principle that some degree of priority access should be given to the people who are building the beamlines and who are bringing resources into the project. At the same time, it was suggested that some sort of “sunset clause” should put limits on the duration of this priority access. It was noted that the current plans call for the beamteams to be peer-reviewed every three years.

It was agreed that at least 25% of beamtime should be made available to “general users” through a peer-review system. If an even higher portion of the beamtime is allocated in this way, such as 50%, then it would be reasonable that beamteam members should have the right to apply for this beamtime as well.

From the point of view of those who will be requesting beamtime in the peer-review stream, the key word is “flexibility”. There is no single type of “general user”. As well, we should avoid dividing users into only two groups, “beamteam members” and “others”.

About half of those present indicated that they would be requesting beamtime frequently. They would prefer to have their project peer-reviewed in a way that would give them access over an extended period, perhaps two years. The other half indicated that they would be requesting beamtime fairly infrequently, and would be happy to apply each time, as long as the process was fast and efficient.

There was some representation from the industrial sector. The comment was made that this sector does not have significant synchrotron experience, and they would be looking for collaborations with the academic sector.

Growing the CLS User community (*Gerald Audette, Nancy Bernini*, facilitators) ~ 15 attended

G. Audette began the session with a brief description regarding the change in focus at the CLS from the production to operation phases, and the need to bring users to the CLS once the facility opens its doors in early 2004. The ensuing discussion focused mainly on the means with which user growth can be promoted in the academic and industrial sectors. Highlights of this discussion follow:

A. Academic Community

1. Encourage cross-fertilization between SR users in Canada. One suggested method is self-promotion by current users in their respective departments and universities, as well as continued promotion by the CLS and the synchrotron institutes.
2. The CLS needs a presence beyond the Canadian chemistry and physics meetings, such as at the Canadian Federation of Biological Societies (CFBS), the Neurological/Neuroscience meetings, the IUBMB meeting to be held in Toronto next summer, etc. This presence can also be used to build connections between the basic and applied sciences, as the Neurologist/Neuroscience meeting brings together basic scientists and physicians.
3. There is a need to show scientists what they CAN do with SR. An analogy: giving a person a fish versus showing them how to fish. Providing the data once is not enough... demonstrating how and what the CLS can do will generate new users in the CLS community.
4. Targeting a "younger" audience: graduate students and post-docs. It was felt that quite often, these younger audiences are more amenable to pursuing the use of different methods / techniques, and are able to bring back their experiences to their home laboratories and departments.
5. Recommendation of the development of a CLS sponsored summer school on SR uses and applications that could be used as a for-credit course towards a graduate degree at participating Universities.
6. SR workshops should be more than just talks - include hands-on experience, as well as social interactions with the SR experts.
7. The CLS sponsorship of a speakers tour, such as has been sponsored by NRCan and several synchrotron institutes (i.e. ASI), would enable allow SR researchers to present the uses & benefits of SR to the Canadian research community.

B. Industrial Growth

Industrial participation & promotion is critical to the CLS, although it is perceived that this will be the hardest area in which to encourage growth. Several ideas for promotion of the CLS in the industrial sector include:

1. Talk to the "front line" people doing the research in industry, in addition to management. This will enable those doing the research to learn the benefits of SR and promote its use internally.
2. Identify current academic/industry collaborations and use these as conduits to industry.
3. Show industry how to solve their problems with SR, and particularly at the CLS, as opposed to simply providing with data from samples that are sent in.
4. Focus on SR use by small to medium sized business, which are a large component of the Canadian industrial landscape.
5. Patience - industry will likely want to see concrete results from the CLS before committing a effort and capital.

The assembled group agreed that there is much work to be done. With patience, promotion and perseverance, both from the community and the CLS itself, the Canadian SR user community will continue to grow.

Phase II beamline procedures (*Tom Tiedje, facilitator*) ~ 30 attended

This meeting was well attended with about 30 people present. The meeting primarily took the form of a fact-finding session with CLS representatives (Bancroft and Hallin) updating the group on the status of the beamline prioritization and planning process that was underway. The meeting was constructive and the input from the CLS representatives was very helpful. The meeting lasted about 45 minutes.

Four beamlines have been approved by the prioritization committee with no priority announced yet. The four approved beamlines are X-ray Emission, Protein Crystallography 2, Double Crystal Monochromator/Microprobe (monochromator being moved from Wisconsin), and the merged Powder Diffraction/Small Molecule beamline. As far as the CLS is concerned the proponents of these beamlines can go ahead and write CFI proposals. The beamline called Vespers (microanalysis/microdiffraction) will go ahead pending approval from the FAC in the new year. A Biomedical Beamline that was formerly rated as not ready to proceed has been moved back onto the active list by a last minute commitment from the U of S to hire a leader for this activity. It is not clear that this commitment will be sufficient in itself to solve the leadership problems in time for the May deadline. It was originally suggested that this beamline would be funded outside the CFI process. No mention of whether this is still the plan. A MEMS (micro-electro-mechanical systems) beamline is being proposed by a U of S group. This has not been approved by the FAC but approval will be sought. The status of this new proposal as far as the CFI application process is concerned, is unclear. No one mentioned the third IR beamline.

Mike Bancroft asked that beamline proposal leaders send copies of their Notice of Intent for the CFI, to the CLS for joint submission to the CFI with a covering memo. The CFI proposals will not all originate from the U of S. Two of the proposals are expected to come from the University of British Columbia. Presumably some or all of the other proposals will come from the U of S but this was not spelled out.

The prioritization committee will rank the beamline proposals. This ranking will be approved by the CLS board on December 5 at which point it will be revealed publicly. The purpose of the ranking is presumably to assist the CLS in setting up a construction schedule for the Phase II beamlines.

The CLS is on record as saying that they will only be able to build "one or two" beamlines a year due to budget constraints. In the worst case this would mean a three-year delay or more for one or more beamlines in phase II. It was pointed out that this would likely be unacceptable to the beamline proponents. Emil Hallin responded to this by saying that the CLS could build two beamlines per year.

