Message from the Director

-Keith Hodgson

The accomplishments of the past year have set the framework and vision for SSRL well into the next century. The upgrade of the storage ring SPEAR has begun, a multi-institutional collaboration on the development of the next generation light source is underway and we have made important additions to our staff and faculty that will strengthen our science and technology programs and user support.

Most relevant to our ability to provide the photons needed for you, our users, to continue to do cutting edge science is the start of the SPEAR3 project (see the separate article that provides more details elsewhere in this Newsletter). Following the successful DOE project review (the “Lehman” review) last summer, the DOE Office of Basic Energy Sciences provided funding through the fall and into the first half of 1999 that enabled us to build up a project team, headed by Tom Elioff, with Bob Hettel as deputy project manager and Richard Boyce as project engineer. In the Fall, DOE and NIH began a discussion that led to an interagency agreement signed in late May that provided framework for funding the project. As a result the first $14M in funds arrived in July.

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From SSRLUO-EC

-Pat Allen / LLNL Chair, SSRLUO-EC

Dear SSRL Users:

This year marks the end of another highly successful run for SSRL. The 1999 run began on an extremely positive note with some of highest lifetimes and vacuum quality readings ever recorded in SPEAR history (see SSRL website for run data). The beam reliability paralleled last year’s performance with an average uptime for the entire run of 93.6%. This continues to be an impressive accomplishment and is a significant source of our scientific productivity. Your Users’ Organization Executive Committee has been actively working on your behalf with the SSRL Laboratory Management Group (LMG) to address many issues that impact users such as: 1) the expanding user base and availability of beamtime, 2) the development of new beamlines and capabilities, 3) maintaining a strong support staff, 4) state-of-the-art computational capabilities, and 5) improving and maintaining user amenities.

On behalf of all the users, I would like to extend our sincere thanks to Suzanne Barrett for all of her help over the last few years. Suzanne recently left SSRL to pursue new endeavors and we want to wish her the best. The users benefited tremendously from Suzanne’s skills at dealing with virtually every facet of SSRL operations, including beamtime scheduling and interactions between the SSRLUO executive committee and the LMG. We also wish to welcome Audrey Archuleta who has recently joined SSRL as the new user administration manager, and are looking forward to working with her in the upcoming years.

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Work is progressing extremely well. An interlaboratory agreement with the Institute of High Energy Physics in Beijing will provide for fabrication of the magnets through an international collaboration and significant progress is being made on all other systems. SPEAR3 is on track for a 2002 installation and will greatly enhance the SPEAR performance to the benefit of all users.

Following up on another recommendation of the Birgeneau-Shen advisory committee, DOE-BES charged another panel, chaired by Professor Steve Leone, to look at opportunities for next generation light sources. Among its recommendations, the panel saw significant opportunity for the linac-based fourth generation x-ray FELs and recommended a focused R&D program that could lead to construction of such a machine in the coming years. DOE-BES has now provided funding for the LCLS collaboration (SLAC, ANL, BNL, LANL, LLNL, and UCLA) to begin a three-year R&D program. A technical advisory committee (chaired by William Colson) and a scientific advisory committee (co-chaired by Jo Stöhr and Gopal Shenoy) have been set up to provide advice and oversight.

SSRL has been very fortunate to attract new and talented staff to our organization during this past year. The SPEAR3 project has been significantly strengthened through the participation of a number of our colleagues from other SLAC Divisions as well as outside the laboratory. We have appointed two new faculty members (Drs. Jo Stöhr and Peter Kuhn) and welcome back Dr. Ingolf Lindau, all of whom will help guide our development in the coming years. Dave Dungan fills a very important role as SSRL Assistant Director for Business and Finance and Audrey Archuleta joins us as head of our user services administration with Suzanne’s departure after more than three years of excellent service and support for the users. Many others have joined other groups in the laboratory as we expand to build the new storage ring, upgrade the beam lines, support a growing community of structural biology, materials and environmental users, and work on the LCLS.

Of course the success of your science depends on SSRL’s performance. As discussed in the article by Suzanne, we continue to support an increasingly large user community. The delivery rate over the most recent 9-month run was 93.6% and the average over the last three 9-month runs has been 95%. The new DOE-BER funded structural biology beam line 9 is now fully operational, the DOE-BES funded environmental science beam line 11 is in commissioning and the new LIGA station BL3-1 has also been commissioned. Many other improvements and upgrades have been made to the other beam lines this past year.

As we look at this remarkable success and plan for the future, it is very important to keep in mind that besides you, the users, and we that run the facility, it is really the funding agencies and their staff that enable this to all happen. It is especially important to note the operations and materials research funding for all of SSRL that is provided by DOE-BES and the efforts of Drs. Pat Dehmer, Iran Thomas, Bill Millman, Bill Oosterhuis, and Paul Smith. The structural biology program is supported by the DOE-BER (the role of Drs. Ari Patrinos, Marvin Frasier, Michael Viola, Roland Hirsch and Charles Edmunds) and the National Institutes of Health (the role of Drs. Judy Vaitukaitis, Marvin Cassman, John Norvell, and Dov Jaron). The SPEAR3 project was advanced through the effort of the OSTP (Dr. Bob Marianelli) and the Directors of the DOE Office of Science (Dr. Martha Krebs) and NIH (Dr. Harold Varmus).

As a Division of SLAC, we also interact with and depend upon many of our colleagues in other divisions here. Over the past 15 years, SLAC has been fortunate to have Burt Richter provide the leadership and vision that has seen the lab (and SSRL) develop. Burt has stepped down as SLAC Director and Jonathan Dorfan took over this role in September. Jonathan has skills in management and vision that will help further strengthen our division’s performance and effectiveness.

As chair of the SSRLUO-EC, I have had a very interesting and busy year. The year began with a meeting of the Science Policy Committee (SPC) which holds semi-annual reviews of SLAC and SSRL. Following this was a meeting of the NRC Committee for Developing a Federal Materials Facilities Strategy. In general, these committees requested input, from a user’s perspective, about important issues that affect users at research facilities. The NRC Committee’s charge was especially intriguing in that they were considering ways of improving or integrating user access at all DOE materials research facilities (i.e., fac...
A Message from the New SLAC Director

- Jonathan Dorfan

As I take on the task of Director of SLAC, I find myself excited by the breadth and excellence of the current scientific program, and enthused by the possibilities for expanding our horizons. In high energy physics, the B Factory has turned on very effectively this June with Babar now running at better than 1/3 of the design luminosity. Our space-based venture GLAST seeks a go-ahead signal early next year as it competes in the NASA Announcement of Opportunity process. R&D towards the next linear collider is making excellent progress.

The growth in the SSRL program in the past five years has been most impressive. SSRL runs a very efficient operation and User satisfaction is high. The scientific productivity is at an all time high and the program has broadened its scientific boundaries with great effectiveness. The near-term outlook is certainly very bright.

But we are not alone in pursuing this science and the competition from other light sources is keen. With the $53M SPEAR3 upgrade, SPEAR will remain a frontier facility well into the next millennium. Inter-agency ventures are increasingly important to the vitality of US science, and I am pleased that the NIH has joined our traditional sponsor the DOE, in support of our future. Equally exciting is the prospect of building the world’s first X-ray FEL facility, the LCLS, at SLAC. This facility could well revolutionize X-ray physics in much the way synchrotron light facilities did. The DOE has chosen SSRL as the lead laboratory for its $4.5M, three year R&D program. Working with our partners, we need to make this program the success that will be needed to generate a construction approval. Equally important for construction approval is the development of clear and convincing scientific arguments for how one can utilize the coherent beams. I am hopeful that the User community will take up this challenge with enthusiasm.

My job as Director is to support the SSRL program to be successful, a task which I pledge to you I will do with gusto. I am making sure that the two future looking programs, SPEAR3 and LCLS, benefit from the best technical infrastructure and personnel that we have available at SLAC. Like PEP-II, SPEAR3 must be built on time and turn on quickly, with excellent early performance. Our program to secure the LCLS for the world user community likewise must be aggressively managed so that we can realize this facility in the not too distant future.

I look forward to meeting you at future SSRL User meetings and forums.

facilities that provide synchrotron radiation, neutron beams, and high-magnetic-field environments to study materials). In addition to discussions with directors of the various U.S. facilities, there were also presentations given by European facility representatives.

The SSRLUO-EC addressed many key issues over the course of the past year. Perhaps the most important of these was the strong recommendation/approval to proceed with the SPEAR3 upgrade. Our input certainly was helpful and SSRL has just received the first stage of funding for the upgrade project. Other topics discussed this year included: implementing DOE-wide computer security measures at SSRL without significantly impacting the user community; the availability (or lack thereof) of affordable user housing; improving the user check-in/check-out procedures; efficient execution of user suggestions received through end-of-run summaries; and issues associated with creating a dedicated SAXS station (BL4-2) while maintaining ample resources to accommodate an increasing demand for molecular environmental science (MES) XAFS stations. Coupled to this last issue, we are now seeing the commissioning of an additional arsenal of wiggler-based beamlines in Sector 11, whose capabilities will encompass MES XAFS (BL11-2) and Protein XRD (BL11-1). So, as we head into the time where SPEAR3 will become a reality, it will be important from a user standpoint to insure that the transition is as smooth as possible and potential delays in our continued scientific progress are minimized. We are looking forward to having a state-of-the art 3rd generation SR user facility which will be well worth the investment of time and money.
SSRL extends a warm welcome to Audrey Archuleta who joined the SSRL staff in September as the new manager of User Research Administration. Audrey has ample experience in the user research administration arena gained from her previous position at Los Alamos National Laboratory. Feel free to stop by and introduce yourself to Audrey in building 120, room 218. You may reach Audrey at (650) 926-3191 or via email at ala@ssrl.slac.stanford.edu.

**User Administration Points of Contact**

- **Beam Time Request Forms**
  - X-ray and VUV
  - Protein Crystallography
  - End of Run Summary Forms
  - Hazards Forms
  - Institutional Use Agreements
  - Proposal Submittal Reviews
  - **Diana Viera**
  - **Daphne Mitchell**
  - **Michelle Steger**

- **Scheduling**
  - X-ray and VUV
  - Protein Crystallography
  - **Audrey Archuleta**
  - **Marjorie St. Pierre**
  - **Daphne Mitchell**
  - **Michelle Steger**

- **User Accounts**
- **User Dosimeters**
- **User Support Forms**
  - **Diana Viera**
  - **Michelle Steger**

The 1998/99 user run (November 2, 1998 - August 13, 1999) presented the SSRL staff with plenty of challenges and opportunities. After some startup problems involving one of the RF cavities, the 40-week user run rapidly came underway, and successfully delivered 94% of the scheduled user shifts. We were able to accommodate the beam time needs of over 280 unique proposals. The SSRL staff scrambled to support 747 experimental starts on 28 beamline stations, a doubling of experimental starts since 1995. Not surprisingly the number of users that arrived on-site to perform experiments also continues to increase with over 782 users being badged and processed through the user research administration office.

Despite our lengthy user run, beam
time assignments remain extremely competitive. When averaged across all beamlines the oversubscription rate was 45% (145% user demand). User over-demand on coveted insertion device beamlines continues to outpace beam availability by 76% (or 176% user demand).

The SSRL user community has grown to nearly 1800 users from over 21 countries. Of the 1296 users on proposals getting beamtime in FY99, 85% were from the U.S. spanning 36 states. These users were predominantly from American universities (59%) followed by American laboratories (21%), American businesses (10%), foreign universities (8%), and foreign laboratories (2%).

On a personal note, I’d like to say thank you to the SSRL staff and user community for all their support and patience throughout my three and half year tenure at SSRL. I have moved to Southern California and

will soon be wrestling with the concept of motherhood. I’ve been advised repeatedly that if I thought managing the user research administration office at SSRL was tough, that I haven’t seen anything yet!

Best wishes,

Suzanne

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**New User Kitchen/Lounge Area on the Experimental Floor**

_Britt Hedman_

SSRL now has an additional kitchen/lounge area for users, this one located behind beam line 9 on the experimental floor in Bldg. 120. It occupies the former Biotechnology XAS Storage Room, which was moved to a new location in the Bldg. 120/131 extension during the 1998 shutdown. The kitchen area provides a refrigerator, a microwave, an electrical range, a sink, kitchen cabinetry for food storage, and filtered, chilled drinking water. The lounge area, which is behind the kitchen area, has been furnished with a generous corner-style sofa, a smaller two-seater (which have already become popular sleeping areas for exhausted protein crystallographers), and two dining tables with chairs. Two areas for computer/network access are being completed during the 1999 shutdown. One will be equipped with an X-terminal, providing access to the central VMS server, beam line computers and NT servers, whereas a Silicon Graphics workstation will enable data backups, as well as access over the network to selected Unix and VMS data acquisition and analysis computers in a second location in the user area.

The funding for the construction of the area, the amenities and furniture was provided by the Department of Energy, Office of Biological and Environmental Research, as part of the beam line 9 operations infrastructure, but is open to all SSRL users as is the rule and philosophy at SSRL. This user area also now ensures that SSRL has a kitchen/user area that conforms to the ADA requirements of access.

SSRL has two additional user kitchen/lounge areas, upstairs in Bldgs. 120 and 131. It was established very late during the construction of these kitchen/user lounge areas in 1997, that the access to the kitchens did not conform to ADA requirements (no elevator access in Bldg. 131; outside access only for the Bldg. 120 kitchen). The construction of the new kitchen/lounge area behind beam line 9 thus also represents the SSRL solution to meet this compliance requirement.

SSRL is very pleased to be able to offer users an additional quiet area away from the high-pace and noisy experimental station areas, with telephone and network connections to enable more private communication with the outside world, and food preparation capabilities around the clock.
SSRL Faculty News

-Gordon Brown, Jr., Chair, SSRL Faculty

I am writing to introduce SSRL users to the SSRL faculty, which currently consists of 11 active members, three emeritus members, and one member on leave. The SSRL faculty was formed in the Fall of 1992, following the merger of SSRL with SLAC, due to the efforts of Seb Doniach and Bill Spicer, the co-founders of the Stanford Synchrotron Radiation Project, and Artie Bienenstock. Seb also served as the first chair of the SSRL faculty, completing his second term as chair in August 1998. The SSRL faculty is a division of the SLAC faculty, which also has a High Energy Physics (HEP) division consisting of 37 regular and emeritus members. The main criterion for appointment to the SSRL faculty is a major commitment to leading the development of a particular research area at SSRL.

SSRL faculty members are of two types: those appointed to tenure-track or research faculty billets with ≥ 50% salary support from SSRL, and those appointed to tenure-track faculty billets in a campus department who are also appointed to a faculty position at SSRL for a term of 3-5 years, which is renewable. Our faculty is recognized as a department by Stanford University, with faculty billets controlled by the Provost’s Office. However, as is the case of the HEP faculty at SLAC, we differ in several important ways from other Stanford departments—we do not grant degrees and we do not teach courses under the SSRL or SLAC banners. The Director of SLAC, Prof. Jonathan Dorfan, serves as Dean of the SSRL and HEP faculties. Lisa Dunn currently serves as the support staff for the SSRL Faculty. Thanks Lisa!

The current SSRL faculty consists of the following members, with affiliations listed in parentheses:

Arthur Bienenstock  Prof., Materials Science & Engineering, Applied Physics, and SSRL (on leave)
Gordon Brown     Prof., Geological & Environmental Sciences and SSRL
Christopher Chidsey  Assoc. Prof., Chemistry and SSRL
Sebastian Doniach  Prof., Applied Physics, Physics, and SSRL
Alice Gast         Prof., Chemical Engineering and SSRL
Martin Greven      Asst. Prof., Applied Physics and SSRL
Keith Hodgson      Prof., Chemistry and SSRL
Paul Phizackerley  Prof. (Research), SSRL
Piero Pianetta     Prof. (Research), SSRL and Electrical Engineering
Z.-X. Shen         Assoc. Prof., Applied Physics, Physics, and SSRL
William Weis       Assoc. Prof., Structural Biology and SSRL
Helmut Wiedemann   Prof. (Research), SSRL and Applied Physics

We also have three active emeritus faculty members: Ingolf Lindau (Electrical Engineering and SSRL), William Spicer (Electrical Engineering, Materials Sciences & Engineering, and SSRL), and Herman Winick (SSRL and Applied Physics).

Two new tenure-track faculty appointments (100% SSRL) were approved earlier this year by the Stanford University Board of Trustees. One is Dr. Joachim Stöhr, who is currently a staff scientist at IBM Almaden Research Center, and the second is Dr. Peter Kuhn, who is currently a staff scientist at SSRL. Dr. Stöhr will join the SSRL faculty as a full professor in January 2000, and Dr. Kuhn will join the faculty this Fall as an assistant professor.

The current SSRL faculty has expertise in the areas of accelerator physics (Wiedemann, Winick), amorphous materials (Bienenstock), condensed matter physics (Doniach, Greven, Shen), molecular environmental science (Brown), polymer science (Gast), structural molecular biology (Doniach, Hodgson, Phizackerley, Weis), and surface science (Chidsey, Lindau, Pianetta, Spicer). The addition of Dr. Stöhr will add strength in condensed matter physics, particularly in the area of surface and thin-film magnetism, and the addition of Dr. Kuhn will add strength in protein crystallography.

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New SSRL Faculty

Two new tenure-track faculty appointments (100% SSRL) were approved earlier this year by the Stanford University Board of Trustees.

**Peter Kuhn**

Dr. Peter Kuhn joined the faculty of Stanford University in an appointment with SSRL in the fall of 1999. He was born and raised in Unterpleichfeld, Germany, and received his Vordiplom in Physics in 1992 from the Julius Maximilians Universität Würzburg. He finished his graduate work at the State University of New York at Albany with a M.Sc. in 1993 and a Ph.D. in 1995 both in Physics after which he joined the Structural Molecular Biology group under Keith Hodgson at SSRL. Dr. Kuhn’s research interests are focused on new methodology and advanced instrumentation for structural biology using synchrotron radiation. He is co-leading the macromolecular crystallography joint with Michael Soltis. Together they carry responsibility for the five beam lines currently dedicated for macromolecular crystallography at SSRL.

**Joachim Stöhr**

Dr. Joachim Stöhr will join the SSRL Faculty in January of 2000. Dr. Stöhr is currently a Research Staff Member in the Science and Technology Department at the IBM Research Division at the Almaden Research Center. Dr. Stöhr received his B.S. in Physics from Friedrich Wilhelms University in Bonn, his M.S. in Physics from Washington State University (as a Fulbright scholar) and his Ph.D. in Physics from the Technical University of Munich. In 1975 and 1976 he was a Postdoctoral Fellow at Lawrence Berkeley National Laboratory and joined the Stanford Synchrotron Radiation Laboratory as a Staff Scientist in 1977. In 1981 he became a Senior Staff Physicist at the EXXON Corporate Research Science Laboratory. He left EXXON in 1985 to join the IBM Almaden Research Center, where he managed various groups, including the Magnetic Materials and Phenomena Department, from 1991 to 1994.

Dr. Stöhr’s research has focused on the development of novel investigative techniques based on synchrotron radiation for exploring the structure and properties of surfaces and thin films. He played a major role in developing surface extended x-ray absorption fine structure (SEXAFS) as a tool for exploring surface structures, especially for adsorbate geometrics on surfaces. He also developed near edge x-ray absorption fine structure (NEXAFS) as a technique for the study of simple and complex molecules bonded to surfaces and for the study of thin organic (polymeric) films. These two techniques have become widely used, and Dr. Stöhr has written definitive reviews of both fields. More recently Dr. Stöhr has turned his attention to the use of x-ray magnetic circular dichroism, XMCD, in magnetic materials.

Dr. Stöhr is the author of the book “NEXAFS Spectroscopy” and more than 200 scientific publications. He is a Consulting Professor in the Electrical Engineering Department at Stanford University, a Consulting Professor at the Stanford Synchrotron Radiation Laboratory, and an Adjunct Professor in Physics at Uppsala University, Sweden. He has been a Fellow of the American Physical Society since 1988.
In addition to the regular faculty, we have two other categories of faculty members who add expertise in other areas – Affiliated faculty and Consulting faculty. The SSRL Affiliated faculty consists of faculty members in other departments at Stanford University who have significant research programs at SSRL. This group is elected to three-year appointments by the SSRL faculty and currently consists of the following individuals: Bruce Clemens (Materials Sciences & Engineering), Roger Kornberg (Structural Biology), Robert Madix (Chemical Engineering), David McKay (Structural Biology), George Parks (Geological & Environmental Sciences, Emeritus), Edward Rubenstein (Medicine, Emeritus), and Edward Solomon (Chemistry). In addition, the SSRL faculty recently elected three new Stanford faculty members to the SSRL Affiliated faculty. These new appointments are Scott Fendorf (Geological & Environmental Sciences), Christopher Garcia (Medical Microbiology and Immunology), and Vijay Pande (Chemistry).

SSRL also draws expertise from outside of Stanford University and SLAC in the form of Consulting faculty appointments. Our current group of Consulting faculty includes the following individuals: Robert Bachrach (Applied Materials), George Brown (U.C. Santa Cruz), David Clark (Los Alamos National Laboratory), Klaus Halbach (Lawrence Berkeley National Laboratory), Albert Hoffmann (CERN), Jack Johnson (The Scripps Research Institute), Steven Laderman (Hewlett Packard), Claudio Pellegrini (UCLA), Douglas Rees (California Institute of Technology), John Rehr (University of Washington), and Joe Wong (Lawrence Livermore National Laboratory).

A Belated Thank You to Seb Doniach

-Gordon Brown, Jr., Keith Hodgson, and Herman Winick

Last year when the SSRL Users Newsletter was being completed, we had intended to include an article on Seb Doniach, the co-founder of the Stanford Synchrotron Radiation Project (SSRP) and first chair of the SSRF Faculty, thanking him for his service to SSRP/SSRL over its entire history and most recently (Sept. 1992 to Sept. 1998) for his service as SSRF Faculty chair. Unfortunately, this article got lost in the shuffle, so we wish to offer Seb a belated thank you for his many contributions to SSRL.

Many of you know Seb by sight - a rumpled guy wearing sandals with a British accent most often seen on his bicycle in transit to or from SSRL. He is also occasionally seen working with his research group at SSRF on BL4-2 on small angle scattering studies of protein folding, although we understand from Seb that his experimental group prefers that he stay in his campus office doing the theory he is so well known for. Some of you may not know that Seb was one of the first (along with his student Charles Ashley) to formulate a modern theory of EXAFS, which was published in 1975 (C.A. Ashley and S. Doniach, Phys. Rev. B 11 (1975) 1279). Seb is now an integral part of the structural biology effort at SSRL and, most recently, the new Initiative on Complex Materials that was spearheaded by Martin Greven, Z.-X. Shen, Bob Laughlin, and Seb.

Back in 1972, Seb Doniach and Bill Spicer had the foresight to found SSRP, with Seb serving as the first Director. SSRP’s first Deputy Director was Bill Spicer, and Herman Winick was hired away from Harvard University to serve as Associate Director for Technical Matters. Ingolf Lindau was a Staff Scientist, and Brian Kincaid and Piero Pianetta were the first two Stanford graduate students to work at SSRP. Seb and Bill prepared a grant application to the National Science Foundation requesting $1.2M for 18 months for construction of SSRP, including the first building and port for the first beamline. They were successful in this initial proposal, receiving full funding, and the SSRP project was completed in 11 months on budget. Seb also had the amazing foresight to conceive of the Participating Research Team (PRT) concept and talked a number of his friends into forming five PRT’s to fund branch lines that utilized the 11 mrad of light from the BL1 port. The five initial BL1 PRT’s were (1) the BL1-1 Grass-
hopper spearheaded by Fred Brown and Bob Bachrach of Xerox PARC; (2) BL1-2 spearheaded by Victor Rehn of the U.S. Naval Weapons Center at China Lake; (3) BL1-3, a hard x-ray XPS Stanford PRT developed by Bill Spicer, Ingolf Lindau, and Piero Pianetta; (4) BL1-4, the “Caltech” small angle scattering PRT line run by Nicholas Webb and John Baldeschweiler for biological studies, particularly studies of muscle contraction; and (5) BL1-5, the original “Bell Labs” XAFS station built largely by Brian Kincaid, with the help of Peter Eisenberger, Dale Sayers, Farrel Lytle, Ed Stern, and Seb Doniach and funded by Bell Labs, Boeing, and the University of Washington. Operation of the SSRP beamlines commenced in May 1974, under strictly parasitic running conditions, and an annual operating cost of ~$300K. All of these branch lines produced remarkable results rapidly, with the first copper metal EXAFS spectrum taken on May 21, 1974. At that time, the SSRP operating budget represented about 1% of SLAC’s annual operating budget (about $30M in 1974); the SSRL operating budget now comprises about 15% of the SLAC annual budget. Based on the phenomenal success of BL1, Seb raised an additional $0.74M in 1975 from NSF to build BL2. In 1976, Seb also spearheaded SSRL’s Phase II funding from NSF, raising $6.7M for construction costs of Building 120, three new BM lines, and one wiggler magnet line. With the success of the first wiggler beam on BL4, the original plans were changed and SSRL built one BM line and two wigglers, plus an extension to Building 120 to house the second wiggler line.

Seb paid careful attention to all aspects of the development of SSRP/SSRL, such as the detailed planning for the first beamlines. He also gave seminars at many universities, companies, and laboratories to spread word about the wonders of synchrotron radiation and the opportunities offered by SSRL in the early days. Perhaps he was too successful in these efforts, as SSRL quickly became overloaded with more users than we could handle, leading to scheduling problems, and then to the Proposal Review Panel. For those interested in more of the early history of SSRP, we recommend the article by Doniach et al. in Journal of Synchrotron Radiation 4 (1997) 380.

From the beginning, Seb made it clear that he would only serve as director in a part-time capacity so that he could maintain his research and teaching activities. When SSRL grew to the point in 1978 that a full-time director was needed, Seb stepped down and Artie Bienenstock assumed the director’s role.

We are fortunate to have a wise and unselfish colleague like Seb who led the effort to build SSRL and conceived of much of the original structure that is still in place. Seb, together with Bill Spicer and Artie Bienenstock, also had the foresight to form the SSRL Faculty in 1992. The SSRL faculty has since played a key role in developing new areas of science and new beamline facilities that have helped keep SSRL at the forefront of synchrotron radiation laboratories. We owe a great deal to this rumpled, sandaled guy with the British accent!

**Awards**

**Martin Greven** was one of six professors at Stanford University to be awarded a Sloan Fellowship for 1997 for his work in correlated electron systems. The Sloan Research Fellowships were established in 1955 to provide support and recognition to young scientists. Martin will receive a $35,000, two-year grant to pursue whatever lines of inquiry he finds most interesting. Greven studies materials physics with an emphasis on advanced single crystal growth, x-ray scattering, and neutron scattering of high-temperature superconductors and materials that exhibit low-dimensional magnetism. Dr. Greven earned his doctorate from the Massachusetts Institute of Technology in 1995 and served as a postdoctoral associate at MIT for two years before coming to Stanford in January 1998.

**Farrel Lytle** was presented with the first SSRL Users Support Award which has been named for him. He was given this recognition for the tremendous service to the SSRL users community he has contributed over the past two decades in a variety of ways, particularly in bringing and introducing new users to synchrotron radiation experimentation, educating, collaborating and assisting users in all aspects of XAFS spectroscopy. With this recognition, Lytle was given a plaque with citation and a check of $1,000.
**Summer Shutdown Projects**

- **Brian Choi, Ben Scott,**  
  **Hal Tompkins and Teresa Troxel**

**Electrical**

Improvements were made to the Meaker bend magnet power supply with replacement of the outdated trigger and regulator circuits by the Power Conversion Department (PCD). An unused magnet bus was removed from the East and West Pit areas to prepare for SPEAR3. PCD also made tests and started implementing improvements of the Booster B2-B6 magnet power supply necessary to operate at 3 GeV for SPEAR3.

**RF Repairs**

In November 1998, the 8S9 cavity, which had given many years of service, exhibited arcing and problems with RF conditioning. Then in March, the high voltage power supply for the 10S11 cavity failed. During shutdown, the 8S9 cavity was disassembled for a thorough inspection of the cells, ceramic window and tuners. Foreign matter was removed, the cells were nitrided and the tuners were cleaned and aligned. This work improved mechanical and electrical control of the drive system. A thorough inspection and cleaning of the 10S11 cavity also took place, and its high voltage power supply was repaired.

**Seismic Retrofit**

SSRL is continuing the seismic retrofit program. The SPEAR control building (Bldg. 117) was one of the buildings identified as seismically inadequate. Since the SPEAR control room is mission-critical to SSRL operations, it was seismically retrofitted during this year’s shutdown. The retrofit work consisted of replacing the existing lateral bracing with stronger bracing, installing new roof bracing, strengthening moment frame connections, adding lateral bracing for the computer control panels and strengthening wall partitions.

**Beam Lines**

Alongside the major projects that have been covered elsewhere in this Newsletter, many of the beam lines received attention as well. The BL1-4 monochromator was pulled from the “coffin” this summer. Radiation-damaged wire was replaced as well as a faulty crystal side slit and crystal bend motion. A new window is also being installed in the back wall of the BL1-4 hutch.

The vacuum hardware associated with the cryostat on BL2-1 has been modified to allow for a faster pumpdown. A new camera has been purchased to allow for easier alignment of the sample holder in the center of rotation of the diffractometer. Software support for the diffractometer slits will be complete by the start of the run allowing them to be controlled from the data collection program (SUPER) resident on the Alpha.
number of spurious trips of SPEAR’s beam.

BL7-3 underwent a major reconfiguration of the hutch area. The experimental hutch has been significantly enlarged, mainly to facilitate use of the new 30-element Ge detector that has been purchased. The electronics racks have been repositioned to allow for a larger space for the experimenter to use outside of the hutch.

Significant changes were made to the BL10-2 electronics racks. The CompuMotor drivers in the rear hutch were completely removed. All but one of the channels had been replaced earlier. The E450’s mounted at the rear of the data collection racks were also removed. This makes access to the back of the NIM modules much easier. The hutch feed-thru panel cables for both hutches were all checked to verify that the data collection rack feed-thru panels were appropriately labeled and the motor driver cables have been relabeled.

The process of replacing the DEC Microvaxes continues on BL10-1 and BL8-1. The necessary motor drivers have been purchased and the necessary ICS code should be completed by the beginning of the user run in November. Users on these beam lines will run SUPER for their data collection.

As mentioned elsewhere in this Newsletter, a new room for SAXS equipment storage adjacent to BL4-2 has been constructed. This required downsizing the Bldg. 131 clean room and the relocation of the gas racks for BL4. So users who wish to check on the gas flow to their ion chambers on BLs 4-1, 4-2, or 4-3 will now visit a new location 20 feet left of the original location. In order to better utilize the more limited floor area of the clean room, loan items such as gaskets and flanges have been moved to the SSRL stockroom.

BL3-3 (aka JUMBO) is undergoing a major revamping of the control electronics that allows peaking of the rocking curve after each motion of the crystal goniometers. The old max-search electronics will be replaced by a programmable controller which will interface with the new Alpha. Users on this beam line will use SUPER for data collection. A new silicon M0 mirror has arrived for BL3-3. Because of personnel limitations, this mirror will be installed during the month of November of this year. This installation requires pulling the mirror tank and setting it up in the vacuum group’s clean room, installing the mirror, baking out the entire system, and finally reinstalling the system after the Thanksgiving holiday. This will require that BL3 remain closed for the first month of the 1999 user run. BL3-3 will have its new hardware and software commissioned in December and will be available to users again in January, 2000.

The new white light LIGA line (BL3-1) will be ready for regular use when BL3 opens again in December. Work on its ventilation system is finished and some small shielding items has been completed.

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**New LIGA Line in Operation**

-Michael Rowen

The new LIGA branch line, BL3-1, was completed and commissioned in July. This white light x-ray line is located on the SPEAR side of BL3-3 and is dedicated to doing exposures for LIGA. LIGA is set of processes to fabricate mini- to micro-scale parts in plastic or metal using lithography, electroplating and molding. A synchrotron x-ray source is ideal for exposing the thick resists of the lithographic step. The new BL3-1 is a white light beam line utilizing 3.4 mrad of the bend magnet source with only beryllium windows and filters attenuating the x-rays. The construction of this branch line has been done in collaboration with Sandia-Livermore and JPL.
**Beamline Projects**

**Beam Line 11**

- Tom Rabedeau

Beam line 11 was a flurry of activity through-out much of the past year. The tempo was set early in the year when the 26-pole, 2.0 T wiggler was installed in the ring along with the associated vacuum chamber during the brief summer SPEAR down. The fast pace continued through design and construction of the 11-0 (beam transport), 11-1 (macromolecular crystallography), and 11-2 (environmental XAS) hutches, design, fabrication, assembly, and installation of numerous optical components, and design, fabrication, and installation of the beam line instrumentation, control, and personnel protection systems. These activities culminated in the extraction of first light on July 20, 1999. But such a brief summary hardly does justice to the developments of the past year, so let’s pick up the thread of the activity following the installation of the wiggler.

Following completion of the wiggler installation, SSRL beam line development and vacuum personnel focused attention on the $M_0$ mirror and associated slit assemblies. The $M_0$ mirrors, which are the first optical elements in both the 11-1 and 11-2 branch lines, provide beam vertical focusing (11-1) or collimation (11-2) as well as power filtering and harmonic rejection. After careful assembly these mirror and slit systems were baked and set aside while the 11-0 optics transport hutch was erected. Following completion of this hutch, the mirrors were installed in the 11-0 hutch in June, 1999.

While the $M_0$ mirrors awaited installation, work progressed on many other BL11 components including the first e-beam welded copper mask employed on SSRL beam lines. This pivot mask utilized fabrication technology developed for SLAC’s high current B Factory vacuum chamber and slated for use on the SPEAR3 vacuum chamber. Like the other BL11 masks, this mask utilized new design concepts and fabrication technologies to meet the thermal challenges presented by the high power of insertion device beam lines on the 500 mA SPEAR3 ring. (Beam line 11 is the first of the SSRL beam lines to be designed for SPEAR3 power loading.)

SPEAR3 power loading poses an even greater challenge for monochromator design. The 11-2 XAS monochromator represents SSRL’s first effort at adapting the...

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*The BL11 insertion device is lowered by crane into the SPEAR ring under the careful attention of SSRL mechanical and vacuum technicians. The magnet assembly and vacuum chamber are identified as the components wrapped in plastic in the center of the photograph.*

*The BL11 front-end as seen at the end of the summer 1998 shutdown. The component at the lower right is a SPEAR dipole magnet. The plethora of hoses conduct cooling water to the BL11 crotch, fixed, and moveable masks as well as a SPEAR quadrupole magnet.*
liquid nitrogen (LN) monochromator technology developed at third generation, high energy light sources for use on undulator beam lines to the demands of high power wiggler beam lines. The 11-2 monochromator features an internally LN-cooled first crystal followed by a contact LN-cooled second crystal. To maximize the beam line operational efficiency, the monochromator includes two such pairs of crystals with a remote crystal change capability adapted from the beam line 9 pinpost monochromator. The 11-2 monochromator, which has been in development since the spring of 1998, was installed in the 11-0 optics transport hutch in August. Initial commissioning studies were conducted during the last several days of the 1999 run and will continue in the fall run.

As of this writing (late September) the long awaited final optical element of the 11-2 branch line, a 1.2 meter, single crystal Si, focusing M₁ mirror, has just been delivered. Over the next several months the 11-2 M₁ mirror system will be assembled with installation scheduled for late fall. User commissioning trials of 11-2 should commence in early winter.

The design and construction of the 11-1 macromolecular crystallography branch line has also progressed well in the past year. As noted above, the M₀ vertically focusing mirror system was installed in June. The design of downstream components is largely complete with most of the remaining 11-1 masks, windows, and filters in various stages of assembly. Like the 11-2 monochromator, the thermal design of the 11-1 monochro-

The branch line 11-2 1.0 meter long, single crystal Si, M₀ mirror and cradle during assembly. The vacuum technicians are installing a Compton scatter shield over the mirror. The side-clamp cooling blocks, identified by the attached copper water cooling tubes, ensure the thermal stability of the mirror system.

The 11-2 M₀ mirror (upward reflecting mirror on the left) and the 11-1 M₀ mirror (downward reflecting on the right) inside the vacuum tank during assembly. The close relative proximity of these two mirror systems is a consequence of multiple branch lines on a single insertion device. The Compton scatter shields prevent each mirror from producing thermal instability in the adjacent mirror.
(continued)

A Si(220) first crystal from the 11-2 LN monochromator. LN coolant flows through two groups of seven holes drilled transversely through the crystal. To reduce the total flow of LN required while maintaining good heat transfer efficiency, each cooling channel is partially filled with an Invar rod. The LN flows only through the annulus formed by the rod surface and the slightly larger diameter cooling channel drilled through the Si crystal.

Installation of the monochromator and the start of 11-1 commissioning is scheduled for the late fall. Design work on the remaining side station of beam line 11 has just started. This side station, 11-3, will feature a vertically focusing mirror with a side scattering, asymmetrically cut monochromator. The station will provide a 10-11 keV fixed-energy focused beam for scattering experiments. First light on this station is anticipated late in the upcoming run.

The 11-2 LN monochromator crystal mount plate as seen during assembly. The two sets of first crystals and attached LN manifolds are denoted “1” while the second crystals are denoted “2”. The path taken by an x-ray beam diffracting from the upper crystal pair is indicated by the arrow. To change the diffraction to the lower crystal pair the crystal mount plate is rotated 180 degrees about an axis normal to the scattering plane and translated such that the crystal pairs exchange positions.

Normal Incidence
Monochromator Beam Line for Ultrahigh Resolution
Photoelectron Spectroscopy

-Changyoung Kim and Michael Rowen

Branch line 5-3 has been one of the most productive beam lines at SSRL. Its main contribution to the scientific community can be found in the area of high-temperature superconductivity (HTSC) research led by Prof. Z.-X. Shen at Stanford. Even though the capability of BL5-3 has been fairly competitive, it has become clear that a system with higher resolution and throughput would be required for future research in this area. The project of adding a Normal Incidence Monochromator (NIM) branch line to the existing beam line was thus conceived.
In the previous two SSRL Newsletters, we reported the design, construction and commissioning efforts of the NIM beam line (BL5-4). Even though the construction was completed and the first beam was brought through in 1997, there were problems remaining that prevented the beam line from reaching design goals. Most notably, due to the delay in grating manufacturing, the monochromator had a sinusoidal profile grating instead of the specified blaze angle grating. This resulted in about three times poorer flux. A second problem was with the first focusing mirror, M1. Ripples on this bendable float glass mirror resulted in the order of a few hundred μm vertical beam size at the entrance slit instead of the expected ~50 μm beam. This forces us either to use large entrance slit sizes hence ruining the resolution or to lose flux.

The first blaze angle grating was delivered in December, 1998. The gas cell test following installation showed an excellent resolution, better than 1 meV and similar to that of the earlier sinusoidal profile grating. The flux increased by a factor of ~3. Two additional blaze angle gratings for different energy ranges are expected to be delivered before the start of the 1999-2000 run. In combination with the state-of-the-art SES200 photoelectron analyzer, the total resolution of the system is about 4 meV as shown in Figure 1 with a gold Fermi edge spectrum taken at 6 K. So far this is the best resolution in the world. With this increase in flux, BL5-4 has been extensively used for various ARPES experiments that could not be achieved before. Figure 2 shows a Fermi surface map of an n-type high Tc superconductor, Nd2−xCexCuO4 obtained by integrat-

![Figure 2. Fermi surface mapping on an electron doped HTSC Nd2−xCexCuO4. The darkest region represents Fermi momentum (courtesy of N. P. Armitage).](image)

Even though the BL5-4 NIM system is already producing excellent data, it does not produce the expected photon flux yet. Figure 3 shows flux measurement results with the 10-period undulator at a 48 mm gap. At the intensity maximum, the flux is about 3.5x10^11 photons/sec/0.05%BW. Calculated flux at this photon energy is about 1x10^12. Therefore, there still is about a factor of 3 difference between the calculated flux and the measured flux. Work is thus underway to improve the M1 mirror. A new polished Si mirror has been purchased and mechanical parts of the mirror bender are redesigned. Installation of the new M1 mirror is expected in October of 1999. With this improved M1 mirror, the flux is expected to increase by a factor of 2 and will then be close to the calculated value.

![Figure 3. Photon flux measurements with the 10-period undulator at 48 mm gap.](image)
New SSRL Facility for Studying Materials in Very High Magnetic Fields

*John Arthur*

In November 1999, a new station will be commissioned for the study of the behavior of materials under very high magnetic fields. The vision for this new station has been provided by Professor Martin Greven who has worked closely with SSRL staff as well as other agencies to secure additional funding. This station is expected to be particularly useful for the study of the so-called correlated electron materials. These materials, usually transition-metal oxides doped with rare-earth metals, exhibit strong interactions among their valence electrons. The electron interactions lead to very interesting bulk properties such as high-temperature superconductivity, colossal magnetoresistance (in which an applied magnetic field can change the electrical resistivity by many orders of magnitude), metal/insulator transitions driven by temperature change, and many forms of magnetic ordering. The detailed mechanisms driving these effects are not understood very well, as they involve a complicated balance of electric and magnetic interactions. Theories are just beginning to

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Integrated Safety Management System at SSRL

*Ian Evans*

Looking to provide a formal and organized process to manage all aspects of Environmental Safety and Health (ES&H) issues at its laboratories, the DOE has developed the Integrated Safety Management System (ISMS). In short, it is a process that allows people to plan, perform, assess and improve ES&H at work. Fundamental to the process are the Guiding Principles that can be viewed as “best management practices”, which are the policies that integrate ISMS at all levels, and Core Functions, which provide the day-to-day tools used to translate policies into something we can all understand.

Guiding Principles:

- Everyone is responsible and accountable for the safe conduct of their own activities, while the supervisor has responsibility and accountability for the protection of employees, the public and the environment.
- That there are clear roles and lines of responsibility, authority and accountability at all levels of an organization.
- That everyone in the workforce has experience, knowledge, skills and abilities to perform their work safely and competently.
- That management allocates resources (money, time, effort) to ensure work can be performed safely.
- That hazards shall be evaluated and appropriately controlled before work is performed to provide adequate protection to employees, the public and the environment.
- That engineered or administrative controls shall be in place to mitigate to acceptable levels work associated hazards.
- That no work will be performed unless it can be done safely.

There are many places in the lifetime of an experimental proposal or during beam time at SSRL, where a user may see the effects of this program. Some may be obvious, such as the SSRL Safety and No-Bars talks, while others are transparent such as the proposal being reviewed for safety considerations, or SSRL’s interaction with outside regulatory agencies. Yet, throughout SSRL (User Operations, Accelerator Operations, User Admin., etc.) the guiding principles are integrated and

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yield predictions which can be tested using x-ray diffraction and x-ray absorption spectroscopy. The ability to subject the samples to a wide range of external magnetic fields, in addition to varying the temperature and modifying the chemical composition, will allow the predictions to be tested over a broad region of parameter space.

The high-field station has been built as an extension of BL7-2. Primarily intended for x-ray diffraction experiments, this new station includes a large diffractometer, which carries a superconducting magnet capable of reaching fields in excess of 12 Tesla. The ability to carry out x-ray experiments on samples under such high fields is almost unprecedented; only one or two comparable facilities exist elsewhere in the world.

The new hutch and diffractometer have been built by SSRL staff during the last six months. The superconducting magnet, a state-of-the-art design by Oxford Instruments, has been purchased using support provided by NSF (M. Greven, P.I.). Prof. Greven’s group will support the operation of the magnet for their research on correlated electron materials, and for other SSRL experimenters who have need for such a high-field facility.

(continued)

applied to all facets of work planning and execution.

Core Functions:

- Define the Scope of Work – The proposal is reviewed to understand the type and nature of the research, to define any ES&H issues or components existing in the proposal, and to effectively deal with them.

- Analyze the Hazard – What are the specific hazards relating to the proposal or its implementation at an SSRL beamline? What controls need to be developed to run this experiment? The Safety Review Summary evaluates and assesses the stated hazards, determines regulatory and compliance needs and proposes solutions to minimize risks allowing for a safe and healthful work place. It is also the mechanism that ties in the User or spokesperson.

- Develop and Implement Hazard Controls – The final controls or mitigating solutions for an experiment are dependent on the degree of risk that that experiment presents. Providing or building a safety system may be a simple or extremely complicated process. Once they have been established, the implementation at the beamline is via the Safety Checklist and Beamline Operations Group.

- Perform Work within Controls – Online and taking data with all safety controls in place and operational.

- Provide for Feedback and Continuous Improvement – As within any system, feedback is a necessity to understand what works and what doesn’t, allowing for real time intervention and assuring that the safety system operates to expectations.

Although we recognize that DOE and other ES&H regulations can be burdensome, taking a systematic and timely approach to hazard identification and mitigation can only lead to a safer environment for all our Users and Staff. The Integrated Safety Management System has a positive affect in how we approach safety issues and how we translate them into good business practices, allowing SSRL to maintain its high standards.
The TXRF Project on Beam Line 6-2

-Sean Brennan & Piero Pianetta

During the past year, the Total X-ray Reflection Fluorescence (TXRF) project on beam line 6-2 has seen significant improvements in minimum detection limit due to the replacement of the focusing mirror on the beam line. By the end of 1996, we had brought our detection limits to 3x10^8 atoms/cm² for transition elements (for comparison, a monolayer is ~10^13 atoms/cm²). This sensitivity is more than an order of magnitude better than TXRF using conventional sources. We can now report a sensitivity of 8x10^7 atoms/cm² for transition metals based on Fe, Ni and Zn standards. This represents a sensitivity of 1 femtogram over the detected area of the wafer surface of 8 mm² as compared to 500 femtograms over a 100 mm² area for a conventional TXRF system.

The TXRF project has been a collaborative research effort between SSRL and a number of industrial partners. The lead industrial associate has been Hewlett-Packard, with Stephen Laderman and Alice Fischer-Colbrie of HP actively involved in the development of the technique. Other semiconductor manufacturers include AMD, Applied Materials, ARACOR, DEC, Intel, IBM, Lucent, Motorola, National Semiconductor and Texas Instruments. The analytical labs involved in the project include Balazs Analytical Lab and Charles Evans and Associates. We have also had university collaborators including groups from the Atomistic Institute of Vienna, Austria, MIT and Stanford University.

The measurement facility is installed in the back hutch of beam line 6-2 and is granted 1/3 of the beam time on that line in a PRT-like arrangement. We have installed a class 1 clean room inside the hutch and implemented an automated wafer-loading robot to eliminate additional contamination to the wafers during the measurement process. For each of our experimental runs the Si(111) crystals in the monochromator are replaced by a pair of Mo-B₄C multilayers which have ~3% band width, greatly increasing the flux on the sample without degrading our elemental sensitivity. The monochromator is typically set to 11200 eV, far enough above the Zn K-absorption edge that the scattered light from the incident beam does not interfere with the Kα and Kβ fluorescence lines from Zn contamination on our standard wafer. The monochromator is tunable, however, and we have studied elements as high as bromine (K-edge=13474 eV), which is often present as a trace contaminant in HF, and we have tuned down below the copper K-edge (8980 eV) to study trace contaminants in wafers covered with that element.

The wafers are installed in a vacuum chamber in a vertical geometry so that the solid state Si(Li) detector can be positioned along the E-vector of the incident beam to minimize the elastic scatter into the detector. Due to the close proximity of the detector to the sample there is still significant scattered light in the detector, and this signal dominates the spectrum collected by the detector. During this past year we have started exploring the use of digital counting electronics, which promises to increase the maximum count rate that the detector can achieve. This will allow us to collect data at the optimum incidence angle (between 0.08 and 0.11 degrees) with a lower detector dead time, increasing the sample throughput significantly.

The other development of this past year is the detection of light elements such as Al and Na, spearheaded by Katarina Baur, a post-doc working in our group. This has been challenging in the past, due to the proximity of the silicon substrate K-absorption edge, which results in large amounts of silicon fluorescence. This fluorescence is diminished on BL6-2 by installing a teflon filter in front of the detector, but such a filter cannot be used for measuring fluorescence from low-Z elements. One can reduce the intensity of the Si fluorescence by choosing an incident energy below that of the Si K-absorption edge, but this does not completely solve the problem, as the Si Kα Raman peak is present even for incident energies several hundred eV below the Si K-absorption edge. Under normal circumstances the Raman peak would be negligible that far below the edge, but because we are attempting to measure very low levels of contamination, the Raman peak is a significant problem. Despite this additional peak in the spectrum, we have achieved a sensitivity to aluminum of 3.4x10^8 atoms/cm², which is much lower than what is achievable with a conventional rotating anode TXRF system. These results are especially encouraging as they were performed on beam line 3-3, which is a bending magnet line with less than 1 mrad horizontal acceptance. If this were done on an undulator, one could expect a factor of 250 more signal without being limited by detector throughput. With such a source a sensitivity for aluminum of 7x10^8 atoms/cm² should be possible. This would be well beyond anything achievable with other methods.
Small-Angle X-ray Scattering for Materials
Science Applications on Beam Line 1-4

- John Pople

Over the past year we have upgraded successfully beam line 1-4 to provide a small-angle X-ray scattering facility focused principally on materials science applications of polymer science and colloidal systems. Studies of novel synthetic dendritic macromolecules and the responses of polymeric networks to macroscopic deformations are among those projects which are awaiting beamtime in the new schedule.

We received a CCD based X-ray detector from Photonic Science in April and, after it was fully commissioned in August, we used the last few days of the beam run to confirm the performance specifications of the device and collect data for users from Johns Hopkins University and Stanford University. The beam line now offers a focused, collimated X-ray source with a flux of $10^{10}$ photons/sec on a spot size which can be focused to a minimum FWHM of $\sim 100$ µm diameter, focused in the vertical plane by a cylindrical mirror. The wavelength is monochromatic, although a slight bend is applied to the monochromating crystal Si(111) crystal in order to enhance the flux and thus the narrowness of $\Delta \lambda/\lambda$ is compromised. The wavelength itself is tunable between the copper and iron edges at 1.38 Å and 1.74 Å (8979 eV and 7112 eV), respectively. After the SPEAR3 upgrade, the flux on BL1-4 will increase by approximately two orders of magnitude, which will greatly enhance the possibility of performing time-resolved studies of polymer dynamics. The detector is a cooled CCD array with a spatial resolution of $\sim 100$ µm. X-rays impinging on the front face of the detector are converted to visible light by a polycrystalline layer of gadolinium oxysulphide scintillator on a fibre-optic substrate. Data are output from the 1024x1024 CCD array at 30 frames per second as 756x581 pixels digital (CCIR) format with 10-bit dynamic range. The maximum beam path from the sample mount to the detector face is 1.67 m, which permits a minimum scattering vector $|\mathbf{q}| = 0.0055$ Å$^{-1}$ (where $|\mathbf{q}| = 4\pi \sin \theta / \lambda$), allowing features up to 1200 Å in size to be observed. A typical scattering range, from $|\mathbf{q}_{\text{min}}| = 0.0055$ Å$^{-1}$ to $|\mathbf{q}_{\text{max}}| = 0.15$ Å$^{-1}$ is demonstrated by the collagen scattering pattern in Figure 1. Data collection and analysis software are PC based, and synchronized with the remote control of the sample environments, detailed below.

For sample environments at this beam line we are currently able to offer the following:

- A four position XY drivable mount for holding solid samples in wafer or pellet form.

- Four purpose built polypropylene inserts to hold small volume (<1 ml) liquid samples in the above mentioned mount.

- A tensile testing device, constructed here at SSRL, (through the efforts of Thomas Hostetter and others), for uniaxial extension of polymer samples (Figure 2). The samples are clamped between two steel jaws in situ in the probe beam in an oven environment with Kapton windows for transmission of the X-rays. The oven temperature can be remotely programmed between room temperature and 120 °C, controlled to within $\pm 1.0$ °C, and the separation of the jaws can be controlled remotely by a stepper motor to extend the polymers up to 120% in length at extension rates between 0.05 and 1000 mm/min. This device has already been utilized on neutron beamlines at NIST, Gaithersburg MD, (using quartz windows for transmission of the beam) to further the insight of the understanding of deformation in elastomeric networks.[1]

- The development of further specialized sample environments, such as shearing cells for polymer fluids and gels, is also underway.

Molecular Environmental Science Developments

- John Bargar and Gordon Brown, Jr.

MES user activities continued to be vibrant at SSRL during the past year. A total of 1749 8-hour shifts were scheduled for hard x-ray and soft x-ray/VUV MES experiments in the 1999 run (Nov. 1, 1998 - Aug. 13, 1999), which is similar to the amount of MES beam time scheduled in 1998 (1759 shifts). Beam line 4-3 was most heavily utilized for MES research, with 457 shifts scheduled for MES experiments (equivalent to 74% of the available time on 4-3 during 1999, a 10% increase over 1998). Examples of MES usage at other SSRL beam lines, as percentages of available time per station, include 62% at BL 4-1 (same as 1998), 30% at 4-2 (14% decrease relative to 1998), 17% at 6-2 (37% decrease), and 19% at 7-2 (36% increase). In total, about 2.7 full-time equivalent beam stations were used for MES measurements in the past season (an FTE beam station is equivalent to the amount of time available on an average beam station during the entire season). The MES community at SSRL is highly multidisciplinary and includes chemists, geoscientists, materials scientists, soil and environmental scientists, civil/environmental engineers, plant biologists, microbiologists, and biochemists. About half of SSRL’s MES users are based at academic institutions, and about half are at DOE laboratories.

MES efforts in the past year have been dominated by the hiring of staff members, instrument acquisition and development, and preparations to commission BL.11-2. Perhaps the most significant development was the hiring of an engineering physicist, Joe Rogers, who will be the beam line engineer and commissioning staff for BL.11-2. Joe comes currently underway. There has also been much activity on the instrumentation front, as one of the most crucial tasks in front of us this year is to instrument BL.11-2. So, what is involved in instrumenting a beam line? The short list of tasks includes: specification and procurement of detectors, including the 30-element Ge array, an LHe cryostat, and furniture for the experimental control area, conceptual design, detailed design, fabrication/procurement, and assembly of a motorized optical rail system for the hutch, optical rail components (including motorized slits, movable fast shutter, calibration foil actuator, and ion chambers), motorized sample positioners, a motorized stand for the Ge detector, a gas mixing/distribution manifold, current amplifiers and high voltage power supplies.

We have made significant progress on each of these tasks. The 30-element Canberra Ge detector array (funded by the DOE Scientific Facilities Initiative (DOE-SFI)) was delivered with its DXP digital signal processing system from XIA, Inc. in November 1998. Initial commissioning (which requires an end station due to the size of the instrument) was performed in January and April 1999 and has shown that the

![MES Community by Discipline](image1)

![MES Community by Home Institution](image2)
detector’s performance exceeds the original specifications (e.g., achieved performance of 280 eV FWHM resolution at Cu Kα and 350 KHz count rate vs. a specification of 310 eV resolution at 200 KHz count rate). We are eagerly awaiting the opportunity to put the detector through its full paces at BL11-2 in the coming year. A requisition for purchase of the 11-2 LHe cryostat system has been initiated, and most of the design/specification work for the hutch instrumentation described above has been completed.

Several other key MES developments, which will benefit many MES users, are underway at SSRL. For starters, we have designed a new sample preparation lab, which will be located in the Building 131 extension, just beyond BL3-3. The lab will house an ultra-clean water system and instrumentation for wet, non-radioactive sample preparation and crystal polishing operations (relocated from the old clean lab in building 120), providing sample preparation facilities for both hard x-ray and soft x-ray/VUV experiments. Another major effort is the design and construction of a spectrometer for grazing-incidence EXAFS, XSW, and reflectivity measurements at SSRL end stations. This instrument will provide significantly improved control of sample positioning (4 axes of motion), 20 scanning, and spectrometer alignment than the current grazing-incidence spectrometer, and is designed to handle samples as small as 1 mm diameter. The latter specification anticipates significantly higher focused fluxes to be delivered by SPEAR3, which will enable measurements on small samples, including crystal faces of natural materials. Detailed design of the spectrometer is progressing well, and we are hopeful that it can be commissioned late in the 2000 run season. Also of note is the anticipated delivery of two solid state detectors optimized for use in the soft x-ray/VUV region (approximately 250 to 4,000 eV). These detectors were also purchased with DOE-SFI funding. One of the detectors is a 10-element Ge array, and the second is a single element Ge detector having an active area of 100 mm². Both detectors will be equipped with DXP signal processors. Each will be windowless, enclosed in bellows for use at vacuum beam lines, and mounted on a motorized slide to facilitate positioning. These detectors should substantially enhance the capability to perform soft x-ray/VUV fluorescence yield measurements on wet samples at SSRL using a differentially-pumped sample cell and protective windows.

With all of these projects under way, users may have to “excuse our dust during construction”. We are looking forward to having a lot to report at this time next year! If you have a chance, please come take a look at the progress on the BL11-2 facilities on your next visit to SSRL.

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### It’s Happening at SSRL

#### Mid-October

**SSRL 26th Annual Users’ Conference**  
October 11-12, 1999

**Small Angle X-ray Scattering Studies at SSRL (Workshop)**  
Tuesday, October 12, 1999

**Workshop on the Fundamentals of X-ray Absorption Spectroscopy Data Analysis**  
Tuesday, October 12, 1999

**11th U.S. National Synchrotron Radiation Instrumentation Conference (SRI’99)**  
October 13-15, 1999

**Workshop on the Science and Instrumentation for the Linac Coherent Light Source**  
Friday, October 15, 1999
Extended Web-based Tools and Resources for Crystallography

The dedicated web-server for the SMB protein crystallography group at http://smb.slac.stanford.edu, was launched in July of 1999 and provides the computational backbone for web-based tools and resources developed for the Protein Crystallography Collaboratory (funded by the NIH-NCRR). A web-based tool has been developed for viewing local diffraction images from a remote location. Safe access is obtained through the normal user’s Unix account via a secure server port. The SMB group also launched the World Wide Beam Lines (WWBL) website at http://smb.slac.stanford.edu/wwb which provides information about macromolecular crystallography beam lines around the world. WWBL is now funded by the NIH and the official site is hosted at the San Diego Supercomputing Center at http://biosync.sdsc.edu.

Beam Line 9-2 in User Operation

The staff of the Structural Molecular Biology (SMB) group of SSRL together with several research groups refined and optimized beam line 9-2 for multi-wavelength experiments. After first light in August 1998, the final end station instrumentation was installed during the early parts of the 1999 run. Experimental commissioning finished in early July 1999 at which time the beam line became fully operational and general users were scheduled during the remaining four weeks of the run.

BL9-2, as part of the beam line 9 project, is funded by DOE-BER with additional support from NIH-NCRR. This center beam line is dedicated to macromolecular crystallography and optimized for the collection of multi-wavelength data for MAD phasing and high-resolution data. The beam line incorporates an upstream collimating mirror, a double-crystal “pin-post” monochromator, and a bent cylindrical refocusing mirror producing a very low-bandwidth, high-intensity x-ray beam. The beam line provides $10^{11}$ ph/s in an energy range of 4 to 24 keV at the sample position. An Area Detector Systems Corp. 2x2 matrix Quantum-4 CCD detector is currently installed on the beam line having a fast readout speed of 10 seconds. A fully computer controlled Huber Kappa goniometer, equipped with X, Y and Z sample translations, allows for simple and efficient alignment of the sample. A detector gantry allows the positioning of the CCD detector in space for a virtual detector size of ~40 x 40 cm². Altogether, the performance and capabilities of this crystallography beam line are excellent.

The diffraction data collected from this station have proven to be of very high quality for successfully carrying out multi-wavelength experiments; our users have reported solving five MAD structures and one molecular replacement structure to date. Of the five MAD structures solved, three were selenium derivatives and two were native proteins that contain iron. Moreover, users report that over 10 additional MAD data sets are currently being analyzed. Data sets were collected from additional derivatives containing Pt, Hg, U and large clusters of metals. Preliminary studies carried out at the L₃ absorption edge of uranium (~17 keV) have provided methods and techniques for making this energy easily accessible and usable for general user experiments. We are looking forward to a very productive user run beginning in late 1999.

Purchase of a Large Area CCD Detector

The National Institute of General Medical Sciences (NIGMS) has funded a state-of-the-art CCD detector to be installed on beam line 9-2. The primary goal of the NIGMS funding is to increase resources and throughput for NIH users as well as...
for general users. We have placed an order with Area Detector Systems Corp. for a Quantum-315 CCD detector. This detector is comprised of a 3x3 matrix of CCD modules (105 x 105 mm² each) for a total active area of 315 x 315 mm² and will be the largest CCD available for general user protein crystallography experiments. The pixel resolution of this new detector is approximately 50 x 50 µm². The combination of large active area, small pixel size and high-speed readout of approximately 1 second, provides a very good match of this detector to the high intensity of BL9-2 and will be ideally suited for the collection of multi-wavelength diffraction data. A multi-processor compute server system and a high-capacity storage array subsystem will be used to handle the large data files (72 Mb each) and high data flow rate. Delivery is expected in the spring of 2000.

**Ultra-high Resolution Experiments on Beam Line 9-1**

Over the last few years we have developed general methods and techniques for collecting ultra-high resolution data (~1 Å and better). General ultra-high resolution data collection equipment and strategies have been developed that employ the use of a short wavelength x-rays (0.78 Å) and a large area MAR345 image plate detector (~345 mm diameter) on beam line 9-1. During the last run, we received 11 proposals for ultra-high resolution projects of which 9 were awarded beam time. Users reported collecting data from more than 15 different complexes at atomic resolution. These ultra-high resolution data sets allow for detailed mechanistic studies, accurate modeling and interpretation of protein-inhibitor complexes and have been used recently for the direct phasing of a 64 amino acid protein.

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**Joint SSRL-ALS Protein Crystallography Workshop on Xenon-Derivatization with the MSC Cryo-Xe-Siter**

On November 18, 1998, a workshop on Xe derivatization of protein crystals using the Cryo-Xe-Siter flash cooling device was co-organized by the Protein Crystallography group at SSRL, the Macromolecular Crystallography Facility at the ALS, and Molecular Structure Corporation (MSC). Over the past few years, the incubation of proteins with the noble gas xenon has been proven to be an effective way to obtain heavy atom derivatives suitable for protein phasing. The Cryo-Xe-Siter, originally designed by scientists at Yale University and made commercially available by MSC, is unique because it enables the production of xenon derivatives and flash cooling of crystals to be done at a constant pressure. The focus of this workshop was to gain hands-on experience using the Cryo-Xe-Siter. The participants were encouraged to bring their own crystals to derivatize in the device and then test by collecting diffraction data. The workshop was held at the ALS at station BL5.0.1.

The workshop began with a presentation by Tim Rydel of the Monsanto Corporation who described his successful experiences using the device as well as the value of xenon derivatives to x-ray crystallographic structure determination. Then after a brief demonstration, the >20 participants each had a turn using the device with their samples or test myoglobin crystals. Most participants found the Xe-Cryo-Siter simple to use. The device obtained a maximum pressure of 300 PSI and conveniently accepted Yale, Hampton and SSRL style pins. Overall, the workshop was successful in demonstrating the usefulness of the device, which would be a valuable addition to protein crystallography experimental facilities.
We completed another successful experimental run in FY99. Scientific projects at the BL4-2 SAXS/D facility included low-angle single crystal diffraction from large unit cell crystals of numerous viral systems and their components; the use of x-ray scattering amplitudes to improve electron cryo-microscopy image reconstruction; time-resolved and static studies on protein folding and molecular chaperons in addition to solution structure studies on a number of proteins and other biological systems. Initial funding for the SPEAR3 upgrade project has now been received and it provides a great opportunity to obtain ideal beam characteristics for SAXS/D experiments on BL4-2. A new wiggler for BL4, which is essential to take full advantage of the low beam emittance of SPEAR3, is in procurement, and will assure high x-ray beam brightness when the SPEAR3 project has been completed. Expected increase in flux density is by a factor of ~80, bringing the brightness level comparable to those at large third-generation synchrotron facilities. In addition, the horizontal beam size will be significantly reduced, improving horizontal small-angle resolution. The new beam characteristics are strongly favorable for time-resolved studies.

Several improvements were recently made to the BL 4-2 SAXS/D facility. The low-resolution single crystal diffraction instrument received a color-video microscope for improved crystal alignment and a motorized vertical translation stage for its goniostat for precise spindle axis alignment. The EMBL gas chamber detector data collection system is now fully operational, and we support EMBL software packages for data processing and analysis. We are in the process of evaluating software suites for processing diffraction data recorded by the image-intensified CCD x-ray detector. A microsyringe-driven rapid mixer, which can work as a flow cell as well, has been built and is being commissioned. This mixer requires much smaller sample volume than what is required for our stopped-flow rapid mixers, though mixing dead time is significantly longer. The Fuji BAS2000 Imaging Plate scanner was relocated to BL4-2 in March so that users do not have to walk over to BL1-5 to scan Imaging Plates. By the time this Newsletter is distributed, we will have completed the construction of a new SAXS/D scanner/storage room adjacent to the BL4-2 hutch to accommodate the BAS2000 scanner and other equipment. Later in FY00 we plan on extending the BL4-2 rear hutch downstream by ~2.4 m in order to house all SAXS/D equipment permanently, eliminating the need of assembly/disassembly of the front hatch equipment upon change-overs to/from SAXS/D experiments. We thus hope to free up a large fraction of time required to set up the SAXS/D facility for increased user beam time. We further propose to combine the standard long camera setup with the short non-crystalline diffraction setup to cover a wider resolution range all the way from ~1000 to ~5 Å without the need of extensive hardware reconfiguration, allowing users to obtain both low and high angle data within a short beam time slot.

Approximately 60% of the total 4-2 beam time was assigned to bio-

-Kirsi Turbedsky (The Salk Institute) mounting a crystal on the low-angle single crystal diffraction instrument on BL4-2 during the SAXS/D workshop in March.
We held two workshops on biological SAXS/D within the last year. The first workshop was in association with the Users’ Conference and focused on recent advances in the field. The second workshop in March 1999 focused on practical issues in data collection and processing for non-crystalline diffraction and low-angle single crystal diffraction.

Lastly, Dr. Melissa Grush has just joined our biological SAXS/D team as a beam line engineer. She brings a strong scientific background in biophysics, and was most recently involved in research and development as well as user support at the Advanced Light Source. Her experience and skills will undoubtedly help accelerate instrumental developments and upgrades, and assure successful user experiments at the BL4-2 SAXS/D facility.

### Workshops on Small-Angle X-ray Scattering and Diffraction in Biology

SSRL hosted a workshop on Small-Angle X-ray Scattering and Diffraction in structural biology in association with the 25th SSRL Users’ Conference in October 1998. The workshop was aimed at giving an overview of solution x-ray scattering and low-angle single crystal diffraction in structural molecular biology. There were 35 registered participants in this workshop, ranging from novice to experienced x-ray scatterers and protein crystallographers. Eight lecturers gave talks about recent developments in solution scattering data interpretation, new usage of the data and low-angle crystallography on large macromolecular complexes.

A second workshop on Small-Angle X-ray Scattering and Diffraction was held in March 1999, a few days prior to the West Coast Protein Crystallography Workshop in Asilomar, in order to complement the first workshop by providing participants an opportunity to conduct short experimental runs on Beam Line 4-2. Workshop participants were encouraged to bring their samples, and over 1/3 of the participants did measure their samples during the workshop.

Participants of the SAXS/D workshop in March discussing data quality of a low-angle single crystal diffraction image just recorded from Kirsi Turbedsky’s crystal on BL4-2. From left are Angel Paredes (Baylor College of Medicine), Jaap Brink (Baylor), Christine Trame (Stanford), Kirsi Turbedsky (The Salk Institute), Xiaping Dai (The Scripps Research Institute), and Hiro Tsuruta (SSRL, with back to the camera).
SSRL Users Newsletter

SMB XAS Beam Line 9-3: Characteristics, Instrumentation and Use

- The SMB XAS Team

Beam line 9-3, the general user side station on the new 16-pole 2T hybrid wiggle beam line 9 dedicated to biological XAS, saw its first user run in 1999. BL9-3 provides extremely high intensity over a broad x-ray energy range, and is designed to provide focused beam from ~4 keV to ~23 keV, and unfocused beam up to ~30 keV. The x-ray optics consist of a vertically collimating 1-m long Rh-coated Si mirror, a double crystal Si(220) pin-post cooled monochromator, and a 1.2 m Rh-coated refocusing bent cylindrical Zerodur mirror (horizontal and vertical focusing). This configuration provides high flux with both excellent energy resolution and good focus.

BL9-3 was put through initial commissioning during the 1998 run, with extensive testing of all optical elements, and definition of the most optimal settings and alignments, obtaining a focal spot of ~0.6 x 4.3 mm. Towards the very last part of the run, the beam line was successfully used for the first XAS experiments including dilute metalloprotein XAS measurements and micro-XAS studies.

The beam line underwent additional optics work during the 1998 Fall shutdown (a new monochromator controller, the addition of an absolute encoder for the 9-motion of the monochromator, an enhanced-flexibility break-out motion for the BL9-2 and BL9-3 beam separation, full motion capabilities of the Mo mirror system). Additional commissioning took place in the beginning of the 1999 run, including the optimization of several user configurations for energy cutoffs and focal properties, and documentation of energy reproducibility and mechanical stability. For the rest of the run it was scheduled for commissioning with users, and later as a normal user run period, with short intervals of SSRL time for additional equipment installation or minor beam line modifications.

The dedicated experimental equip-

It was Shula Jaron, Oregon Graduate Institute (member of the N.J. Blackburn group) changing sample in the BL9-3 hutch during a commissioning run. In the foreground is the LHe cryostat into which the sample, at the end of the cryostat rod to the right, is being inserted. In the background is seen the 30-element Ge detector array.

ment on BL9-3 includes a Canberra 30-element Ge detector array for which the windowing is computer controlled (high-level software developed at SSRL) with windowing files saved and restored when moving from element to element. It also has a LHe cryostat system, a computer-controlled motorized optical rail supporting ion chambers, computer-controlled motorized beam slit systems, an in-hutch shutter to protect the sample, sets of attenuators, foil holders, etc. Integrated with the rail is a motorized detector alignment carriage that allows for remote exchanged in minutes.

Although this station is formally a side station, the optical configuration of BL9-3 and BL9-2 (the end station, whose beam pipe traverses the BL9-3 hutch) was carefully designed such that the BL9-2 beam pipe location allows for a near end-station configuration for BL9-3. It is thus feasible to utilize two fluorescence detectors, one on either side of the sample, for certain experiments, and there is room for the installation of other equipment, like a single crystal goniometer, imag-
ing/tomography equipment, or a grazing tomography instrument. Two dedicated DECAlpha stations are in use at the beam line for data acquisition (ICS and XAS-Collect) and analysis (EXAFSPAK and FEFF).

During the final phase of commissioning, and during the user commissioning period, it has become apparent that the design goals have been met and that the quality of the data being achieved is remarkably good. The typical focal spot used is ~0.6 x 4 mm FWHM, with a measured flux of ~2.5x10^{12} ph/sec/100 mA at 9000 eV, with no pre- or post-monochromator slit apertures. With a 1x4 mm hutch slit, the flux at the focus (i.e. at the sample) was measured as 8.1x10^{11} at the same energy/current.

Several user groups were scheduled simultaneously on BL7-3 (the second dedicated biological XAS station) and BL9-3 to allow direct comparisons of data quality, collection times, and characteristics of the two beam lines. Continued characterization by SMB staff and improvements based on feedback from these user experiments/experimenters have proceeded in an interleaved fashion. The first publication of data from the commissioning phase has appeared in print and numerous data sets are currently undergoing analysis.

BL9-3 has several inherent advantages over BL7-3 as a result of the optical design, each contributing to significantly greater flux delivered to the sample. For BL7-3, harmonic rejection is provided by detuning the second monochromator crystal, typically rejecting 40-60% of the flux. The BL9-3 vertically collimating harmonic rejection M_0 mirror, when adjusted to the proper energy cutoff, allows the monochromator to be fully tuned, maximizing the flux. As the tuning is maximized to the relatively broad top of the rocking curve, this furthermore reduces the risk for tuning shifts on the steep rocking curve sides that can result in large changes in flux during a scan and be a potential source for noise. The measured flux on BL9-3, using focused beam unapertured in the hutch, is ~7x greater than that for BL7-3 with the both monochromators fully tuned. Under typical SPEAR2 running conditions, with the BL7-3 monochromator detuned 50% and BL9-3 fully tuned, and with a respective typical beam aperture of 1x15 mm and 1x4 mm, the flux is ~10x higher for BL9-3 at the sample.

A significant amount of commissioning time was devoted to establishing optimized hardware configurations for a series of energy cutoffs. As all optical elements are under computer control via the ICS software, these configurations have been stored, resulting in only minor adjustments after they are recalled and the optics are set to these values when moving from one mirror cutoff to the other. The M_0 mirror also reduces the thermal load on the monochromator, the thermal stability of which is further enhanced by having the branch line stoppers located after the monochromator. This, in combination with excellent monochromator and overall mechanical stability, has produced an observed energy reproducibility per shift of 0.055 eV at 10.2 keV.

The collimation of the M_0 mirror removes vertical divergence, resulting in a very parallel beam incident on the monochromator crystals, and thus enhanced energy resolution, without the need for a narrow vertical aperture before the monochromator. We have observed excellent energy resolution (FWHM of the KMnO_4 pre-edge feature <1.65 eV) with the full beam on BL9-3. Finally, the BL9-3 focusing M_1 mirror concentrates the photons into a small spot, allowing physically smaller samples to be measured without sacrificing photon flux, making a very significant enhancement, for example, for combined XAS-Mössbauer samples cells, allowing for small sample quantities, and enabling single crystal XAS measurements.

The data quality obtained on BL9-3 is excellent! Data were measured by the R.A. Scott group (Univ. of Georgia) to k=13 Å^{-1} for a 0.5-mM frozen solution of a Zn-containing protein yielding acceptable data in a single scan using the 30-element Ge detector and a Soller slits/Cu filter setup. The N.J. Blackburn group (Oregon Graduate Institute) was able to measure a complete data set from a 0.3 mM Cu-containing protein in 8 scans, for which acceptable data could not be achieved in a reasonable time on BL7-3. In fact, SSRL staff and the user groups have observed that to collect data of equivalent quality on the same sample on each beam line typically requires about ten scans on BL7-3 for each scan on BL9-3. This effect is even greater for samples whose physical size limits the useable beam on BL7-3 (which is an unfocused beam line with typical beam size 1x15 mm, equipped with a 13-element detector), such as spe cial cells we have developed, which fit into a Mössbauer spectrometer as well as the XAS cryostat. With these cells the beam is limited horizontally to about 4 mm resulting in a ratio of >20:1 for the number of scans required on BL7-3 relative to BL9-3 for equivalent data on dilute Fe protein samples.

In a study of Cu samples of known concentration we have collected useful data down to a concentration of 100 μM, and the R.A. Scott group has found that “analyzable Zn EXAFS data can be obtained with a single 21-min scan on a 0.18 mM
protein sample on BL9-3”. In fact, where on BL7-3 there is a practical limitation on concentration due to the lack of fluorescent signal, the current limitation on BL9-3 for the most common elements (Mn, Fe, Cu, Ni, Zn) could well be background fluorescence from trace amounts of these elements in cryostat materials, sample holders, sample buffers, etc., which will be addressed. The ability to collect data at lower concentrations was recognized by several user groups as an important new capability allowing a new range of experiments approaching physiological conditions.

The increased signal-to-noise has also meant that high-quality data can be measured to an extended k-range, which increases the resolution of the EXAFS measurement, allowing better determination of individual bond distances and helps in reducing correlation problems in the EXAFS curve-fitting analysis. It is also worth noting that the effects of monochromator glitches are eliminated or significantly reduced at BL9-3, possibly as a result of the harmonic rejection mirror.

The greatly increased flux of BL9-3 in combination with the 30-element array detector will thus result in higher throughput and signal-to-noise for “average” samples, extend to lower concentrations the limit to which data can be collected, and enable new experimental capabilities for very small samples to take place. We are moving full speed to develop capabilities for new applications including polarized protein single crystal studies, micro-XAS and micro-tomography for biological materials, and look forward to a very productive year at the beam line in continued pursuit of learning new capabilities as well as testing the limits.

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**SPEAR3 Upgrade Project Is Underway**

- Bob Hettel

After the landmark signing of a Memorandum of Understanding between the Department of Energy and the National Institutes of Health for the joint funding of SPEAR3, engineering and design for the $53.1M upgrade project was authorized by the Basic Energy Sciences division of the DOE to begin on June 1, 1999.

Full project authorization commenced July 17 when the first $14M, provided by the NIH, was received at SLAC. In fiscal year 2000, an additional $15M is expected from the NIH with the remaining funding to come from the DOE in fiscal years 2001 and 2002.

SPEAR3 photon focused flux density (Figure 1) and brightness will be one to two orders of magnitude greater than for SPEAR2 due to the lower emittance.

![Figure 1. Focused flux density for SPEAR2 (100 mA) and SPEAR3 (500 mA) for BL 10 insertion device and a bending magnet beam line.](image)

| Table 1. Accelerator and beam parameters for SPEAR2 and SPEAR3 |
|-------------------|-----------------|-----------------|
|                   | units           | SPEAR2          | SPEAR3          |
| Energy            | GeV             | 3               | 3               |
| Emittance, with IDs | mm-rad          | 160             | 18              |
| Current           | mA              | 100             | 500             |
| Lifetime          | h               | 40 @ 100 mA     | 18 @ 500 mA     |
| Critical energy   | keV             | 4.8             | 7.6             |
| Circumference     | m               | 234.126         | 234.126         |
| RF frequency      | MHz             | 358.53          | 476.34          |
| Harmonic number   | -               | 280             | 372             |
| Injection energy  | GeV             | 2.3             | 3               |
| ID source $\sigma_x / \sigma_y$ | $\mu m$ | 2000 / 53      | 427 / 30        |
| Dipole source $\sigma_x / \sigma_y$ | $\mu m$ | 790 / 200      | 160 / 50        |
| Bunch length      | mm              | 23 (75 ps)      | 5.3 (19 ps)     |
reduced from 160 to 18 nm-rad, and higher beam current, increased from 100 to 500 mA. Accelerator and beam parameters for SPEAR2 and SPEAR3 are compared in Table 1. The improved performance will be attained by replacing the storage ring magnets, magnet power supplies, vacuum chamber, RF system, and by 500 mA with those beam lines closed. The full benefit of 500 mA SPEAR3 operation will be realized at the completion of an independent beam line upgrade program. The upgrade plan includes replacing the electromagnet wigglers for BL4 and BL7 with permanent magnet devices, and installing a 4-m undulator optimized for the 1-4 keV spectral regime and having a brightness of \(\sim 10^{10}\) (photons/s/mm\(^2\)/mrad\(^2\)/0.1% BW) at the 1.5 keV fundamental energy, comparable to the brightness found at other 3\(^\text{rd}\) generation light sources.

The SPEAR3 design has advanced significantly over the last year, thanks to an expanded design team implementing improved instrumentation and control systems [1, 2]. Beam lifetime is calculated to be 18 h at 500 mA, with the 9 A-h lifetime quality factor (the product of instantaneous lifetime and beam current) remaining roughly constant as the beam current decays over the course of a fill. Beam fill times will be reduced and fill-to-fill orbit reproducibility will be maximized by injecting beam at the full 3 GeV operating energy, eliminating the present need for ramping ring energy from 2.3 to 3 GeV after filling.

The main ring installation is scheduled for a 6-month period beginning in April, 2002. Since some beam lines will not have been upgraded for full 500 mA operation by 2002, SPEAR3 will operate initially at a lower current (~200 mA), although it will be able to operate at that includes many experienced engineers from SLAC. Design concepts have evolved and for some systems differ substantially from those presented in the 1998 SPEAR3 Conceptual Design Report, particularly for the RF and vacuum chamber systems.
The revised project funding of $53.1M includes installation of a new RF system capable of supporting 500 mA operation instead of using the existing system, which would only support 250 mA. Four new single-cell, mode-damped copper RF cavities (Figure 2), like the ones developed for the PEP-II B Factory, will be installed together with two new 650 kW klystrons to provide longitudinally stable beam operation up to the full current. The 476.3 MHz cavity frequency permits the ring circumference to remain unchanged and is sufficiently close to the 476 MHz PEP-II frequency to require only minor changes to the cavity design. A minor change in the magnet lattice matching cell design provided the 1 m increase in straight section length to accommodate the 7.5 m needed to group the four cavities in the West pit.

PEP-II engineering expertise also led to an improved vacuum chamber design. Instead of the formed stainless steel design envisioned a year ago, the chamber will be machined from copper (Figure 3). The water-cooled copper chamber will be passively safe for dipole radiation beyond 500 mA, and will be protected from mis-steered insertion device radiation for beam currents above 20 mA by an orbit interlock. Instead of being fabricated in Europe, as was the case for the stainless steel design, the copper chamber will be machined locally and e-beam welded at SLAC, enabling much tighter control over the fabrication process and removing it from the project’s critical path.

Other design changes include decisions to replace the existing concrete magnet support girders with new steel girders, to install a new cable plant system outside the ring shielding, to improve tunnel shielding and thermal insulation properties by installing concrete roof and wall sections that completely enclose the pit areas, and to provide more LCW for the SPEAR site. As recommended by the 1998 Lehman Review Committee, the new magnet girders will be pre-assembled with magnets and vacuum chambers prior to installation in the tunnel to ensure meeting the 6-month schedule. The new cable plant will also help speed the schedule since much of it can be installed outside the shielding before the 6-month downtime.

Meanwhile, rapid progress has been made on the design of the SPEAR3 magnets, which is proceeding in collaboration with the Institute of High Energy Physics (IHEP) in Beijing with a considerable cost savings for the SPEAR3 project. The precedence for this collaboration was set during the PEP-II project, for which IHEP successfully built the Low Energy Ring magnets. After visits to Beijing by SPEAR3 managers and magnet engineers (Figure 4), an international collaborative
agreement was signed by SLAC and IHEP directors in March 1999, and IHEP engineers arrived at SSRL in June to participate in detailed magnet design. Design packages for dipoles, quadrupoles and sextupoles were all completed in September, and magnet material procurement commenced. The schedule calls for delivery of the last magnet, complete with magnet measurement data, before October of 2001.

The designs, costs and production schedules for these and other SPEAR3 systems, including power supplies, instrumentation and controls, and conventional facilities, were examined by technical and management experts during the DOE semi-annual review held on September 14 and 15, 1999. The technical review panel included John Galayda (APS), Alan Jackson (LBNL), Brian Kincaid (LBNL), and John Noonan (APS). The review was chaired by Jim Carney from the DOE Construction Management Support Division, and included DOE representatives Bill Franzwa and Hanley Lee from the SLAC site office, Bill Oosterhuis and Paul Smith from the BES headquarters in Germantown, MD. Marvin Cassman and John Norvell from the National Institute of General Medical Sciences, and Abraham Levy from the NIH National Center for Research Resources attended the review sessions held on the first day.

The conclusions of the DOE review were overwhelmingly positive, with solid endorsements for all major design decisions and some suggestions for further investigation into girder design and reducing the effects of diurnal temperature excursions. The committee emphasized the need for a detailed and integrated 6-month installation schedule, and for the development of contingency plans in the event of project funding or production schedule delays. These suggestions will be addressed in more detail at the next semi-annual review in the Spring of 2000. The review panel was particularly impressed with the solid commitment to the success of the SPEAR3 project by Keith Hodgson and Jonathan Dorfan, the new SLAC Director, who has given the project high priority at SLAC and will continue to make available manpower and facility resources as needed.

With design and management expertise, funding, and interagency commitment to the success of the project in hand, it’s full steam ahead for SPEAR3!

References:

1. SPEAR3 Design Report, draft revision 8/31/99; final version to be published in Fall 1999.


Figure 4. SPEAR3 representatives (left-to-right from center: T. Elioff, R. Boyce, D. Dell’Orco, and N. Li) meeting with IHEP magnet designers and accelerator staff in Beijing in March 1999.
The LCLS

-Max Cornacchia

Several significant events took place in the past year that added momentum and credibility to the Linear Coherent Light Source project. The collaboration was extended to include Brookhaven National Laboratory and Argonne National Laboratory, thereby considerably strengthening the design group, which now encompasses SLAC, ANL, BNL, LANL, LLNL, and UCLA.

It was reported in the last Users Newsletter that the BESAC panel on synchrotron user facilities, chaired by R. Birgenau and Z.-X. Shen had recommended, in 1997, funding for research and development of fourth generation sources. The DOE Office of Basic Energy Sciences (BES), following this recommendation, set up a panel, chaired by Professor S. Leone to make specific recommendations on the development of a path towards fourth generation sources. The Leone subgroup gave its report to BESAC earlier this year. Among its recommendations, it encouraged a focused program of R&D that could lead to construction of an x-ray R&D facility (the LCLS) and identified this spectral region as offering the best scientific promise.

The DOE has announced a commitment to begin this multiyear R&D program in FY 1999. With this support, the LCLS collaboration is undertaking a program that will address a number of technical objectives important to the successful operation of LCLS. Given suitable progress in the next two to three fiscal years, construction could start as early as FY 2003 with commissioning and operation three years later. A conceptual design report will be produced in the spring of 2001.

The following is a short reminder of the layout and major characteristics of the facility. A photoinjector will be used to generate a bright electron beam. Bunches of electrons (one bunch at the repetition rate of 120 Hz) are accelerated and magnetically compressed from an initial length of 10 psec to a final one of 280 fsec. After acceleration to 14.3 GeV in the last 1/3 of the SLAC linac, the beam is transported to a 100 m long undulator, where the FEL radiation is generated and channeled to an experimental area. The transport system and the undulator area use an existing tunnel that presently houses the Final Focus Test Beam (FFTB).

The projected peak brightness of the FEL radiation is 10 orders of magnitude above existing radiation sources. Accompanying this FEL radiation, and independently of the lasing action, the spontaneous radiation that will be produced has high bandwidth, comes in sub-pico-second long pulses and is four orders of magnitude above existing sources. This leap in performance is possible because of major technical advances in some of the experimental tools of high-energy physics and synchrotron radiation. These are the development of

Acknowledging SSRL Sponsors

It is very important that users of SSRL acknowledge the sponsoring agencies that make this resource available. SSRL submits several annual reports to the Department of Energy and the National Institutes of Health which require up-to-date publications listings. These publications lists are extremely important in presenting our scientific achievements and productivity, and thus funding case to these agencies. Users and staff are asked to submit two copies of each publication or thesis based, fully or partially, on work at SSRL to the attention of Lisa Dunn. A reference submittal form is available for users and staff to provide reference information in advance of the actual preprint distribution at the following url:

http://biosg1.slac.stanford.edu/admin/form_publications.html

For both staff and users the correct acknowledgment which must appear in the publication is:

> Work done (partially) at SSRL, which is operated by Stanford University for the Department of Energy, Office of Basic Energy Sciences.

All biology users (except protein crystallographers) and materials and environmental EXAFS users should add the following:

> The SSRL Structural Molecular Biology Program is supported by the National Institutes of Health, National Center for Research Resources, Biomedical Technology Program, and by the Department of Energy, Office of Biological and Environmental Research.

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> The SSRL Structural Molecular Biology Program is supported by the National Institutes of Health, National Center for Research Resources, Biomedical Technology Program, the Department of Energy, Office of Biological and Environmental Research, and the National Institutes of Health, National Institute of General Medical Sciences.
(continued)

LCLS Conference

The need to attract potential users and to explain to them the extraordinary properties of the LCLS radiation is receiving increasing emphasis. On January 12-14, 1999, a workshop was held at SSRL with about 90 participants to address scientific opportunities with the LCLS. It was clear that the scientific discoveries enabled will be evolutionary (i.e. experiments now marginal on a 3rd generation source will become feasible), revolutionary (in the femtosecond time domain and with full transverse coherence) and extraordinary, where creativity and imagination will produce new science not yet conceived.

One class of experiments will be pump-probe, where a modified state is created and then probed on the femtosecond time scale with the LCLS x-ray pulse. New areas in chemical physics, structural biology and material science will open up for dynamical structure studies. The coherence can be used for holographic imaging at atomic resolution. Optimism was expressed at the possibility of achieving holograms with a single x-ray pulse, paving the way for real-time studies of structural charge distributions. A contaminated cathode is the suspected cause of the non-uniform electron beam and therefore a new cathode will be installed in September 1999. The GTF will start operation again when the SSRL injector linac begins operation in October 1999.

The exploration of the parameter space of the LCLS continued, with a view to reduce the risk factor in some of the specifications. It appears possible to reduce the charge in the bunch of 1 nC of the Design Study to as low as 0.1 nC if the emittance decreases with beam current as the simulations predict. A reduction of the electron charge per bunch would reduce phase space dilution due to wakefields. A theoretical study of chirping the FEL radiation shows that the LCLS has the potential of producing pulses as short as a few fscc.
**Some of the Visitors to SSRL this Year**

**Australian Delegation**
A group in Australia is proposing to build a synchrotron radiation facility there to better serve their growing user community, now consisting of several dozen scientists who travel abroad to use several of the 45 sources in operation in other countries around the world. Five Australian scientists visited SSRL on September 1 to learn about the latest applications of synchrotron radiation and the plans to rebuild the SPEAR ring to meet third generation source standards. They were greeted by SLAC Director Burt Richter who urged them to plan for an electron energy in the several GeV range to produce hard x-rays, which are essential for the increasingly important applications to structural molecular biology and molecular environmental science. Various options that may be considered by the Australians, ranging from starting their program by purchasing a small superconducting 700 MeV ring as a turn-key operation from industry to going immediately to a higher energy and possibly replicating a 2.5 GeV ring now in construction in Germany.

**Canadian Delegation**
SSRL hosted eight representatives of federal and provincial Canadian governments, university leaders and economists in a day-long session about the scientific and economic benefits of a synchrotron laboratory. If a Canadian lab is approved, it would be built in the province of Saskatchewan. After its information gathering, the Canadian team will submit its recommendations to the national government in the fall and if approved, ground breaking could occur as early as April, 1999. The present design for the 2.9 GeV Canadian light source is similar in many ways to the design being developed for the SPEAR3 project, so as both of these new facilities progress there is likely to be interaction between the two groups.

**LCLS Collaboration**
There were three visiting scientists at the GTF this summer. Dinh Nguyen from LANL, Dave Dowell from Boeing and Massimo Ferrario from INFN in Frascati Italy. Dinh and Dave are two of the best photo-injector experts in the world and they came to collaborate on experiments at the GTF. The goal was to measure the electron beam emittance using a temporally shaped laser pulse but the experiment had to be delayed due to commissioning problems with the new laser.

Massimo has been using the HOMDYN code that he developed to optimize the beamline parameters to produce the minimum emittance out of the photo-injector.

**Chinese Visitors**
SLAC and the Institute of High Energy Physics (IHEP) in Beijing, China have signed an Inter-Laboratory Collaborative Agreement (ICA) for the construction of the main magnets for the SPEAR3 project. In early July of this year, four Chinese colleagues came to SSRL to help in completion of the designs for the Gradient Dipole, Sextupole and Quadrupole magnets. These engineers will continue their excellent work through the end of October during which time they will return to China and oversee the fabrication and measurement process for the magnets. The group leader, Huamin Qu, and his three colleagues, Yun Yang, Hao Yu and Rui Hou, have worked steadily since their arrival and to date we have completed the Gradient Dipole design and are well along with the other two designs. The IHEP administrative representative, Janling Jiang, also visited SSRL for several weeks and during his stay our two laboratories completed and signed the Attachments to the ICA which forge the final agreements for cost and schedule for the production magnets. The overall schedule calls for prototype magnet completion in early 2000 and full magnet production release by mid 2000.

**Deputy Director of the Shanghai Synchrotron Laboratory**
Professor Zhao Zhentang, Deputy Director of the Shanghai Synchrotron Radiation Facility and professor of accelerator physics, visited SLAC from August 9-13 as part of the US/PRC Cooperative Agreement. While here he gave a talk on the Shanghai project. In visiting SLAC he was particularly interested in the PEP-II central control room, PEP-II high power RF system and low level RF system, lab set-ups for PEP-II beam instrumentation and vacuum system, and in the SPEAR injector (LINAC and Booster), insertion device and beam lines. While here, he made full use of his time in discussing the operation with SSRL faculty.

**Boris Battenman**
“Bob” Battenman was the founding director of CHESS at Cornell and has interacted with SSRL on a technical and scientific level for over 20 years, having also been on the SSRL Proposal Review Panel for 10 years. He is currently the Walter S. Car-
penter Professor of Applied Physics at Cornell and Director Emeritus, CHESS. As of January 1 of this year he is on half time status at Cornell and has come to SSRL and ALS with a research grant to pursue studies with micro-x-ray beams and their application to materials problems.

**Claudio Pellegrini**

Prof. Pellegrini spent the month of August at SSRL to help with the studies of the Linear Coherent Light Source. He will spend several months of the year at SSRL in the next few years to contribute to the R&D program of the LCLS. Prof. Pellegrini is a UCLA physics professor and leads the FEL Physics effort of the LCLS. He is a recent winner of the Free-Electron Laser Prize, assigned each year by an international committee to researchers who have made outstanding contributions to the field.

**Till Helmut Metzger**

Dr. Metzger from the University of Munich, Germany spent 3 months at SSRL earlier this year. He has been a collaborator with us for a number of years on an “X-ray Diffuse Scattering Investigation of Defects Introduced by Ion Implantation in Silicon.” In the course of this work we have discovered a unique signature of planar defects as opposed to point defects and point defect clusters. This allows us to separate the two different defect classes and follow their annealing kinetics as a function of temperature. The experimental work was done at Beam Line 7-2. Work to perform a detailed kinetic analysis is continuing and should receive considerable impetus from an additional post-doc who will join this project early next year. The scientific findings from this investigation should have a significant fundamental impact as well as be of importance technologically.

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