SSRL Strategic Plan

April 2007

The mission of SSRL is to "*enable and support outstanding scientific research by a broad user community in a safe environment*." Throughout its more than 30-year history, SSRL has indeed embraced this mission and has become famous for its supportive and safe environment and for the development of many x-ray techniques and instrumentation that are now routinely used around the world to address grand challenges in many scientific disciplines.

1. The SLAC Environment and General Considerations

SSRL's strategic plan is embedded into the larger transformation of SLAC, which is rapidly evolving into two main areas of scientific focus: Photon Science (PS) and Particle & Particle Astrophysics (PPA). By 2009 SLAC will be devoting both of its operating accelerator facilities, the SPEAR3 storage ring and the LINAC, to Photon Science. This transition is supported by the Office of Basic Energy Sciences within the DOE's Office of Science.

It is the goal of SLAC and Stanford University to become the world's leader in the new multidisciplinary field of Photon Science, the study of matter through its interaction with photons. Photon Science at SLAC is founded on two forefront x-ray sources, SPEAR3 and LCLS, operated as general user facilities. These National Facilities with thousands of general users will be increasingly complemented by SLAC/Stanford based Centers of Excellence, which explore the use of photons to solve grand scientific challenges. Several such Centers are envisioned. The first two Centers, called PULSE (for Photon Ultrafast Laser Science & Engineering) and XLAM (for X-Ray Laboratory for Advanced Materials), have already been established. We envision others such as a Photon Science Center for Energy and the Environment, and a Center for Structure, Function, and Dynamics of Biomolecular Machines. These Centers are designed to take full advantage of SPEAR3 and LCLS, as well as future photon sources at SLAC, and emphasize the multidisciplinary use of photons for scientific advancements. An Accelerator Science Center is also envisioned to develop frontier photon sources that will continue to enable new science. This center will capitalize on the outstanding accelerator physics talent at SLAC and the significant resources, such as the 2 km of linac not used for LCLS and the PEP-II facility as well as developing new concepts for photon sources.

SSRL, founded in 1972, is one of the pioneering synchrotron facilities in the world, known for its strong user support, a "lean and mean" operation, and its close coupling to the science programs at Stanford University, which is driven by the intellectual leadership of the SSRL Faculty in various scientific fields. The goal of SSRL has always been to be "famous for enabling scientific research and producing scientific accomplishments". The facility is well known for pioneering contributions in new synchrotron methods and instrumentation and the new science these enable. Examples of important developments are:

- X-Ray Absorption Spectroscopy (XAS) Techniques: EXAFS, SEXAFS, NEXAFS
- MAD (multiple wavelength anomalous dispersion) phasing
- Soft X-Ray Science (200 – 3000 eV) (Grasshopper, Jumbo monochromators)
- Synchrotron-Based Photoemission Techniques (core level photoemission, photoelectron diffraction, and ARPES)

- Wigglers and Undulators
- Coronary Angiography
- Magnetic Microscopy with X-Rays
- Utilization of X-rays for Molecular Environmental & Interface Science (MEIS)

While SSRL caters to a broad range of users, one may point to certain areas of scientific excellence for which SSRL is famous and which are producing world-class science. It is important for a facility to identify and support selected areas of scientific excellence which help differentiate it from other facilities. SSRL's main areas of scientific excellence are:

- Structural Biology/Chemistry – local atomic coordination and bonding, macromolecular crystal structure, conformational structure of biological assemblies, nanoscale structure.
- Correlated and Magnetic Materials – high T_C materials and oxides with nanoscale ordering phenomena, magnetic materials and magnetic nanostructures.
- Molecular Environmental Science – chemical bonding, oxidation states, micro- and nano-structures and compositions, interaction of organic matter and microorganisms with solids.
- Surface and Interface Science – surface reactions, catalysis, chemical and biological processes at liquid-solid interfaces.

A new area under development is Energy Sciences, which is concerned with the exploration of materials and processes for the generation and storage of energy.

Future developments at SSRL over a 5-10 year time frame are based on the SPEAR3 storage ring, which in 2003 replaced an older source. The new ring is of intermediate energy (3 GeV) and offers high brightness x-ray radiation, which is emitted as short (about 30 ps) x-ray pulses. These capabilities allow the development of new instrumentation such as x-ray microscopy and scientific applications in areas such as nanoscience. More generally, it will become increasingly important in the future to create micro- or nano-sized x-ray beams with high-intensity, well defined polarization and time structure. Studies using such beams promise unique insight into the properties of the following systems:

- Materials that are artificially nanostructured or intrinsically inhomogeneous on the micro- and nanoscale.
- Biological crystals that only exist on the microscale.
- Systems containing interfaces between solids, microbial organisms, organic matter, and aqueous solutions and water in confined spaces under ambient conditions.
- Materials under extreme conditions, such as high pressure, high temperature, or high fields.
- Materials that exhibit nanoscale dynamics, i.e. respond to excitations or naturally fluctuate on the second to picosecond time scale.

We review the status of SSRL's beam lines and facilities in Section 2, address developments that are funded and currently under way in Section 3, and present new unfunded capabilities which are planned for the future in Section 4.

2. Status of SPEAR3 – An Intermediate Energy, Third Generation Source

SSRL, a Division of SLAC, utilizes x-rays produced by the Stanford Positron Electron Asymmetric Ring (SPEAR). The original storage ring was replaced in 2003 by a new "third-generation" ring, referred to as SPEAR3, resulting in one of the world's leading sources for photon science research. It is envisioned that SPEAR3 will be able to serve the research needs of a growing number of national and international scientists across a range of science, engineering, and biomedical disciplines for years to come. The strategic plan outlined here is for the full utilization and optimization of SPEAR3 for x-ray science over the next five years or so. Underlying SSRL's strategic plan is the firm conviction that storage ring based synchrotron radiation sources will remain the workhorses for x-ray based research in the foreseeable future. In contrast, Linac based sources like LCLS, while offering unprecedented opportunities for discovery, will serve a smaller, more specialized user community.

Presently there are 11 beam lines on SPEAR3. The 7 insertion device and 4 bending magnet beam lines serve (in 2007) 27 experimental stations, 20 of which can operate simultaneously. Three additional stations are currently closed for upgrade or cannot be supported due to the lack of staff. SPEAR3 offers great future opportunities since only half of the total 14 insertion device source points and only 4 out of the possible 18 bending magnet source points have been utilized. Part of the SSRL strategic plan is therefore based on the implementation of new state-of-the-art beam lines. Below we list the current status of all SSRL beam lines.

Status of beam line upgrade program (red = insertion device (ID) beam line)

BL1: 95% ready for 500 mA, one out-of-alcove mask needs to be analyzed. (*2 stations: materials SAXS; macromolecular crystallography*)

BL2: 500 mA capable. (*2 stations: powder diffraction, microprobe XAS and "standard" XAS*)

BL3: Shut down. Beam line available for future developments.

BL4: Existing SAXS BL4-2 runs with new wiggler – but limited to <100 mA. BL4-1 and 4-3 not illuminated by new ID. Beam line to be rebuilt in new location in 2007 with the 3 stations. (*1 station currently: biological SAXS*)

BL5: 500 mA capable. (*3 stations: coherent soft x-ray scattering, PES/XES, ARPES*)

BL6: 500 mA capable. (*3 stations: XAS/XES, microprobe, hard-x-ray microscope*)

BL7: 500 mA capable after completed upgrade in 2006-2007. User program resumed on BL7-1 and BL7-2 in February 2007. BL7-3 open for general user program. (*3 stations: macromolecular crystallography, materials scattering, biological XAS*)

BL8: 500 mA capable. (*3 stations: PES, PES, XAS/PES*)

BL9: 500 mA capable. (*3 stations: macromolecular crystallography, macromolecular crystallography, biological XAS*)

BL10: 500 mA capable. (*3 stations: XAS/PES, XAS, materials scattering*)

BL11: 500 mA capable. (4 *stations: macromolecular crystallography, MEIS XAS, macromolecular crystallography, materials scattering*)

In summary, 86% of IDs and 75% of BMs are 500 mA compatible.

3. Present SSRL Developments

Before outlining the strategic plan for the future, we shall briefly discuss developments that are currently under way. These are:

- Completion of SPEAR3 compatible beam line upgrade program
- New beam lines and facilities under construction – BLs 6, 12, 13, and 14
- Accelerator development of 500 mA operation and top-off injection
- Increase of user support by additional staff
- Modes of operation with reduced pulse length

3.1 Completion of beam line upgrade program

The remaining major tasks for the beam line upgrade program are upgrading/rebuilding BL4 and moving/re-establishing 2-5 keV XAS (BL6-2 and BL3-3/JUMBO capabilities) on a new station.

BL4 is being rebuilt in a new location in order to maximize beam time available to users, and provide optimum performance. In this way, installation of the new BL4 will begin during the 2007 run in the new location with entirely new hardware. The permanent magnet wiggler, which is identical to the BL7 wiggler and was fabricated and installed specifically for SPEAR3, will be moved during the 2007 summer shutdown, allowing the new BL4 to be commissioned beginning in the fall of 2007. The new beam line will include the same functions: 4-1 and 4-3 will be optimized for XAS (one station will include capabilities down to 2.1 keV) and 4-2 will continue to be used for biological small angle scattering.

A few minor tasks related to masks and slits on BL1, BL8 and BL10-1 also remain. These latter tasks do not require significant resources and will be completed during FY2007.

The JUMBO monochromator and BL3 have been decommissioned. A new station will be developed on BL14 which will provide new facilities in the 2-5 keV x-ray range. This beam line is also mentioned in the next section and will be commissioned in the fall of 2008.

3.2 New beam lines and facilities under construction

BL12: Advanced macromolecular crystallography beam line, optimized for challenging studies (weakly diffracting crystals, ultra high resolution and large unit cells) and microcrystal experiments
Funded by the Gordon and Betty Moore Foundation through Caltech
60% general user facility
In-vacuum small gap undulator source
Nominal beam size: 20 µm x 200 µm, Intensity ~ 3 x 10^{12} ph/s
5 x 5 μm^2 apertured beam, Intensity ~ 4 x 10^{10} ph/s
Commissioning to be completed in first half of 2007

BL13: Soft x-ray microscopy, scattering, advanced spectroscopy beam line
Funded by DOE-BES
Variable polarization soft x-ray undulator on order,
BL 13-1: STXM sidestation, presently under design
BL 13-2: Photoemission and x-ray emission station, to be moved from BL5

BL 13-3: Coherent soft x-ray scattering station, to be moved from BL5
Commissioning in fall 2007

BL14: BL14-1: High-throughput macromolecular crystallography station
Funded by Genentech and JCSG, with end station equipment from BL1-5
(unless additional funds are identified). Commissioning in fall 2008
BL14-3: soft x-ray XAS (2-5 keV) focused and unfocused
Funded by DOE-BER & DOE-BES, end station equipment from NIH NCRR
Commissioning in fall 2008

BL6: BL6-2: Hard x-ray transmission x-ray microscope
Funded by NIH NIBIB
Instrument purchased from Xradia, Inc.
Instrument located in a new third hutch on BL6-2
Commissioning initiated Dec. 2006

3.3 Accelerator development of 500 mA operation and top-off injection

Part time operation of SPEAR3 at 500 mA is planned for late 2007 when most of the beam lines will have been upgraded for high current running. The storage ring itself has been run several times at 500 mA with beam lines closed during special machine studies periods since June 2005. Stable operation at high current is accomplished by tuning rf cavity control parameters and by increasing chromaticity using sextupoles to suppress multibunch instabilities. The beam lifetime is nominally 14 h at 500 mA, but can be reduced or increased following adjustment of the vertical beam size. While a significant rise in temperature of some vacuum chamber components was measured, no rise was beyond tolerable levels. The electron orbit was measured to be highly stable with feedback at high current, although a true assessment of beam stability at experimental stations must wait until beam lines are open.

With a 10-15 hour lifetime at 500 mA, the beam will decay to 325 mA over the 8-h fill period presently used for 100-mA operation. In contrast, the 100-mA beam only decays by 15 mA in this time. Not only is the heat load on optical components five times larger at 500 mA than at 100 mA, but the variation in that load over 8 hours dwarfs the present value and is likely to be a dominant source of beam parameter instability for experiments. An even greater thermal load transient occurs when beam line radiation stoppers are closed and reopened for injection, as presently required by the radiation safety system, thus completely removing and restoring full beam power on optical components.

To reduce the variation of high-current heat load on optical components, SSRL is implementing top-off injection. The first phase of this operational mode will be to inject new beam on top of an existing stored beam with beam line stoppers open, thus avoiding the large thermal transient on optical components caused by closing the stoppers during injection. To accomplish this mode, SSRL must first receive approval to do so from the SLAC Radiation Safety Department, which would be granted only after significant analysis and review, and then modify the radiation safety system to ensure that it is safe for personnel on the experimental floor. These steps are anticipated to be complete during 2007.

Once beam can be injected with beam line stoppers open, the time interval between injections and the thermal load on optical components can be reduced at the cost of more frequent potential interruption to experimental data acquisition. SSRL will work to establish the optimal period between fills that maximizes beam stability and data quality for users given the performance limitations of the injector. The demands on injector stability, reliability and the speed at which it can be turned on become more stringent as the refill interval decreases. A program is already underway to improve injector performance so that the refill interval can be reduced to 10 minutes in 2008, enabling a stored current constancy of ~1% at 500 mA, and to the order of 1 minute in 2009, yielding a 0.1% current constancy in SPEAR3.

Work has also begun to study the effects of the injection transient on various beam line experimental systems so that a more quantitative evaluation of the optimal top-off operation mode can be made. It is expected that some data acquisition systems will be immune to the injection transient, while others will have to be gated at that time. In some cases, the detector systems might be synchronized with the injection repetition rate so that the transient has no effect. SSRL will work closely with the user community to arrive at top-off operational modes that are of maximum benefit.

4. SSRL Strategic Plan for the Future

SSRL's strategic plan for the next five years is the full utilization of the capabilities of the SPEAR3 storage ring for synchrotron radiation research, coordination of the user program with that of LCLS, and planning for the period past 2012. This involves the following key elements:

- Improvements of SPEAR3 beam lines and instrumentation
- Continued excellence in current areas of strengths, such as structural molecular biology, correlated and magnetic materials, molecular and environmental science, and surface and interface science
- Generation of new facilities that reflect key areas of scientific focus of the user community
- Extension and improvement of user administration and support, jointly for SSRL and LCLS
- Formation of a task force to plan for new x-ray sources at SLAC

4.1 Improvements of SPEAR3 beam lines and instrumentation

Specific emphasis will be placed on new detectors, where collaboration with other SR facilities and detector development groups, detector manufacturers, and with other SLAC Photon Science programs will focus on providing high-performance detectors optimized for the specific experiments and accelerator/beam line performance. For XAS, detectors for high-, soft- and low-energy experiments, such as high-element, fast monolithic solid state detectors are funded for SMB and proposed for MEIS/materials research. High-sensitivity large-area detectors for biological SAXS are under development and procurement with detector manufactures, and fast detectors for time-resolved SAXS are funded. PSD detectors for macromolecular crystallography will continue to be pursued through collaborations, and area detectors for microdiffraction in materials science are planned.

Materials science diffraction beam lines will be reconfigured and optimized for diversified specific science–driven instrumentation, including optimized detectors, sample environments, and diffractometers.

Microprobe capabilities will be tailored to specific scientific areas, ranging in spot size from macro to nanometer scale. Approaches will include capillary-based (BL9-3); Kirkpatrick-Baez based (BL6-2 & BL2-3); Kirkpatrick-Baez based optics in the 2-5 keV region XAS (BL14-3); hard x-ray microscope (BL6-2); and STXM (BL13).

Automation in beam line optimization and data acquisition will be developed where appropriate, and remote-access user experimentation (as at present for macromolecular crystallography) will be implemented in other areas; in-situ monitoring with non-SR techniques will be implemented for sensitive biological and other samples.

4.2 Continued excellence in current areas of strength

Structural Molecular Biology:

The Structural Molecular Biology (SMB) program develops technologies, instrumentation and methodologies in macromolecular crystallography, x-ray absorption spectroscopy and small angle x-ray scattering/diffraction. It disseminates these for use in the biomedical research community, and operates 9+ beam line stations that support a large user community. Current and planned initiatives capitalize on the enhancement in SR performance resulting from the new SPEAR3 accelerator, and focus to optimize the SMB facilities to take full advantage of SPEAR3's increased brightness.

Ongoing and new initiatives build upon novel instrumentation, including advanced detectors, technique-specific software and automated/high-throughput systems for a range of applications. These include the study of high-resolution structures of large, complex macromolecules, including molecular machines; imaging the spatial distribution and chemical nature of elements in non-crystalline biological materials; investigating fundamental questions in biophysics such as protein and RNA folding; and developing and improving methods for the determination of electronic and geometric structure for non-crystalline biological materials at atomic resolution.

The scientific developments are facilitated by parallel developments in software to provide expanded capabilities for instrument and detector control, remote data collection and real-time data analysis. Relevance is to a number of important biological problems including the structure of enzymes, metalloproteins, membrane-bound proteins and immunoglobulins; the active site structure of metalloproteins involved in oxygen metabolism, nitrogen fixation, and photosynthesis; and how these structures change in different states or evolve in time as reactions or events like protein folding or conformational changes occur. Such information is more broadly important to the health-related areas of drug design, cancer research, and virology. The SMB program is supported mainly by DOE BER, NIH NCRR, and NIH NIGMS.

Correlated and Magnetic Materials:

Today, the properties of complex materials, especially materials that exhibit charge and spin order on nanometer length scales or are artificially structured with nanoscale dimensions, form the central theme of modern condensed matter physics. Examples of materials in bulk form are transition metal oxides like the manganites and cuprates whose properties have led to a paradigm shift in our thinking about the structure and electronic properties of matter. Examples of nanostructured materials are artificially engineered magnetic materials, often in the form of simple metals or alloys, with nanoscale size in at least one dimension.

The study of such materials requires forefront and often even the combination of the most sophisticated x-ray methods to distinguish inhomogeneities in atomic structure, chemical state, crystallographic structure, electronic structure, spin structure and temporal structure. At SSRL we are developing improved and new soft x-ray capabilities for such investigations, such as angle resolved photoemission, soft x-ray microscopy and coherent scattering facilities. We will increasingly emphasize the temporal nature of phenomena, in particular equilibrium dynamics and the material response to excitations, such as infrared, optical or field pulses.

Molecular Environmental & Interface Science:

Interfacial, molecular, and nano-scale processes control the toxicity and bioavailability of contaminants and the cycling of nutrients in the environment. Frequently, environmental reactions are further mediated by the formation, dissolution, and migration of complex natural materials such as biofilms and biominerals, including narrow band-gap semiconducting nano-oxides and nano-sulfides. These processes and materials are poorly understood, in general, but are of enormous significance to global biogeochemical processes, such as carbon sequestration and element cycling.

Basic and applied MEIS research at SSRL focuses on the molecular-, nano-, and electronic structures of these complex systems and the chemical and biological processes affecting them at molecular and nanoscales. *In-situ* measurements are a necessity because of the importance of water and the mechanical/chemical complexity of these systems. The photon-in/photon-out nature of synchrotron techniques and the richness of the structural and electronic information they provide make them uniquely suited for molecular environmental and interface science. MEIS investigations at SSRL are performed using bulk and micro-beam synchrotron x-ray absorption spectroscopy (XAS), wide-angle x-ray scattering (WAXS), small-angle x-ray scattering (SAXS), x-ray standing wave (XSW) spectroscopy, and photoemission spectroscopy (PES). Research in these areas is critical to the development of cost-effective contaminant remediation technologies, accelerated clean-up of contaminated DOE sites (such as the Rocky Flats Environmental Technology site near Denver, Colorado), improved storage of high level radioactive waste, the discovery of novel nano-semiconductors for energy sciences, improved understanding of heterogeneous catalysis in systems containing aqueous solutions, and improved understanding of the environmental reactivity of materials used in advanced nuclear systems.

The SSRL MEIS program supports ongoing user research activities and develops new user instrumentation and methodologies in x-ray absorption spectroscopy and x-ray scattering/ diffraction. Current foci include the commissioning of a 2-µm hard x-ray microprobe (funded by DOE-BER-ERSP), and an *in-situ* x-ray scattering chemical dynamics program. Future instrumentation projects will include the development of a STXM microscope that covers the “intermediate” x-ray energy region (200 eV to 10 keV) with an advanced environmental chamber for environmental and biological studies. Research efforts will emphasize themes crosscutting between energy and environmental sciences and ultrafast science.

4.3 Generation of new facilities

Over the last few years, the upgrade of SPEAR2 beam lines has been SSRL’s highest priority in the development of experimental facilities. In addition, the financing of selected new beam lines, listed above has been secured and these are now under construction or being commissioned. In parallel, SSRL has held various workshops to define the need for new beam lines and experimental facilities. The recommendations from such workshops were presented by SSRL management to several external review committees, like the June 2003 Director’s Review Committee, chaired by Sunil Sinha and Russ Chianelli, the February 2005 BES Major Facilities Review Committee, organized by Pedro Montano, and the July 2006 Scientific Advisory Committee (SAC) review. Furthermore, the SSRL User’s Organization Executive Committee

(SSRLUOEC), the SSRL Proposal Review Panel (PRP), and the Structural Molecular Biology Advisory Committee (SMBAC) were continuously involved in the planning process. Through this planning process the following plans for new facilities have emerged. Funding for these is presently being sought.

4.3.A. High-resolution Photoemission Beam Line

We propose to build a new undulator-based photoemission beam line with variable polarization, covering the photon energy range of 10 – 150 eV on one of the existing straight sections at SSRL. This is the spectral range where valence band and shallow core level photoemission spectroscopy can be best performed. We also propose one permanent endstation that integrates spin-resolved capability with ultrahigh resolution angle-resolved photoemission spectroscopy (ARPES). The proposed facility features several capabilities that are either rare or unique among the existing synchrotron facilities in the US, enabling new classes of science that otherwise can not be done. Among these unique capabilities are:

1) excellent control of the polarization over the entire energy range with an elliptically polarizing undulator, an important feature for both ARPES and spin-resolved photoemission experiments;
2) a beam line with two branch lines that combines a grazing incidence monochromator with a normal incidence monochromator (current beam line 5-4), offering great flexibility in choosing between high flux and high resolution based on the nature of the experiments;
3) a dedicated photoemission system that is capable of performing both high resolution angle-resolved photoemission and spin-resolved photoemission experiments in the same experimental chamber;
4) a sophisticated material synthesis chamber that attached to the ARPES system enables synchrotron based experiments not possible otherwise.

The proposed beam line will cover a critical spectral range that is currently not available at SSRL. The existing NIM beam line at SSRL has been very successful, but its limited energy range (10 – 30 eV) makes it difficult to perform angle-resolved photoemission experiments in higher Brillouin zones – an area of increasing importance, to accommodate shallow core level photoemission experiments, resonance photoemission or absorption experiments at transition metal 3d and rare earth 4f edges, and to discriminate surface from bulk electronic states. Moreover, the NIM beam line is already approaching its ten year anniversary and an upgrade is needed to stay at the cutting edge.

Scientific motivation:

As complex and nanoscale phenomena are becoming the central theme of modern condensed matter physics, high-resolution photoemission spectroscopy has gained prominence, as exemplified by its impact on the high-T_c superconductors. Over the last decade, the improved resolution and carefully matched experiments have been the keys to turn this technique into a sophisticated tool for the investigation of complex phenomena. With extremely high angular and energy resolutions achievable these days, this technique reveals the electronic structure with unprecedented precision and sophistication - information which forms the foundation for a comprehensive understanding of complex solids.

Looking towards the future, the field will continue to develop at the breathtaking pace we have seen over the last decade. There will be a continued push for even better resolution in both energy and momentum, and to apply it to an even wider range of problems. Substantial improvement in the quality of the materials is also expected, and systems with extremely low dimensionality, where this technique has unique advantages, will grow in importance, as some of the very interesting physical phenomena occur in these systems. At the same time, concerted efforts will be made to perform angle-resolved photoemission experiments with spin detection, and to perform experiments with very high spatial resolution approaching the molecular level. These improvements will open new frontiers with opportunities for new discoveries and surprises.

In contrast to the rapid improvement of the energy and momentum resolution of the electron spectrometers, the development of state-of-the-art synchrotron radiation facilities has lagged behind. Existing beam lines in the US can not fully capitalize the scientific opportunities presented by the advances in the spectrometers and sample improvements. In this regard, the SPEAR3 upgrade at SSRL provides us with a golden opportunity to make progress in this direction by developing a high resolution, high brightness synchrotron-based photoemission facility.

4.3.B. Small Angle X-ray Scattering Beam Line for Materials Sciences

The proposed beam line will be used for both small angle x-ray scattering (SAXS) and wide angle x-ray scattering (WAXS). The emphasis of the research on this new beam line will be real-time, dynamic studies of materials with a variety of sample environments available (furnaces, stop-flow cells, grazing incidence). The beam line is based on a bend magnet source with a spectral range of 5.9-15 keV. Horizontal and vertical focusing will be performed with a 1.2 m toroidal Ru coated mirror. The focused beam size will be 0.5 mm (horizontal) by 0.3 mm (vertical). Since anomalous SAXS is important to the planned science program, the x-ray energy will be easily tunable. The monochromator will have the capability for Si(111) crystals (high resolution, anomalous) and multilayers (high flux). There will be one hutch with the capability for simultaneous SAXS-WAXS with multiple detectors. A 50cm x 50cm area detector is planned for SAXS, while a curved wire detector is planned for WAXS. This will cover a **Q** range of less than 0.01 to about 60 nm^{-1}. The available sample environments will include furnace (up to 800 ^{o}C), solution cell for 0-100 ^{o}C, multi-sample holder, and giSAXS setup.

Scientific motivation:

The proposed, new beam line is necessary because of the large demand from our users for SAXS and for simultaneous SAXS/WAXS. It will complement the existing SAXS beam line 4-2 which emphasizes biology. The new beam line is motivated by the importance for many materials of obtaining structural information over a range of length scales often in real time during materials processing or other reactions such as synthesis and catalysis. The beam line is further motivated by the importance of *in-situ* studies in surface, environmental and chemical sciences. Many of the opportunities for real-time studies have recently become available from the increased flux densities available at the SSRL source as a consequence of the SPEAR3 upgrade.

The anticipated science includes *in-situ* studies of the synthesis of metallic alloy nanoparticles used as catalysts in fuel cells and of the corrosion or structural degradation of these nanoparticles during catalysis; *in-situ* studies of the phase transformations and catalytic processes during hydrogenation/de-hydrogenation reactions of hydrogen storage materials under controlled temperature and pressure; investigations of changes in the particle size and structure of the bioxides UO_2, goethite, and MnO_2 under reaction conditions (mimicking the natural environment); studies of phase transitions in block co-polymers and supramolecular assemblies; real-time studies of pore formation during processing of nanoporous films templated from copolymers; grazing incidence (surface sensitive) SAXS studies of nanoporous films used a templates and of mineral surface reactions; *in-situ* studies of the flocculation of titania-based colloids (paints); and investigations of phase separation in metallic glasses. The research projects mentioned above are largely supported by DOE Basic Energy Sciences (BES) and are central to the BES mission. The new beam line will facilitate the success of these research programs and will have a significant impact on this research.

4.3.C. Inelastic X-Ray Scattering and Advanced Spectroscopy Beam Line

We propose the construction of a beam line for medium resolution (~ 0.2 – 2 eV) inelastic x-ray scattering and advanced spectroscopy in the 4.6-17 keV range. The proposed undulator beam line will be located at the upstream straight section of the SPEAR3 east pit chicane. It will have dedicated instrumentation to routinely perform high resolution photon-in photon-out spectroscopy including non-resonant x-ray Raman scattering (XRS), resonant inelastic x-ray scattering (RIXS), selective x-ray absorption spectroscopy (S-XAS) and x-ray emission spectroscopy (XES). Two dedicated instruments are proposed for the beam line a) a multi-crystal backscattering spectrometer for XRS operating close to the vertical plane, and b) a multi-crystal tunable spectrometer for RIXS, S-XAS and XES operating close to the horizontal plane. Furthermore we will develop dispersive x-ray optics for single shot and pump-probe XRS, XES and RIXS experiments which can also be used in future experiments at LCLS. The insertion device and instrumentation up through the front end will be funded by SSRL. Prototypes of the analyzer instrumentation are currently under development with internal funding. We will request funding for:

i) a double crystal monochromator with two *in situ* crystal sets for low and high resolution (Si(111) and Si(311))
ii) x-ray focusing optics which in conjunction with apertures provide a variable beam size ranging from 10x10 μm^2 to 1x2 mm^2
iii) beam transport high power masking and slits and associated vacuum equipment
iv) control electronics, machine and personnel protection systems, experimental hutch, experimental hutch tables, and control area infrastructure
v) analyzer instrumentation that ensures an efficient and flexible use of the beam time

In contrast to some of the very high energy resolution techniques, which require high brightness, the proposed techniques rely in principle on a large focused flux density. High focused flux density implies a source which simultaneously provides good flux and brightness which is well matched to the source parameters of an undulator located in the east pit chicane of the SPEAR3 ring. With SPEAR3 operating at 500 mA, the beam line will provide a focused flux of order 10^{13} photons/sec/eV, comparable to best existing beam lines. It will be equipped with novel analyzer optics with unprecedented efficiency currently under development at SSRL.

Scientific motivation:

The beam line will uniquely profit from and complement the existing research programs at SSRL, in particular its extensive and longstanding program on x-ray spectroscopy. It is expected to serve a broad group of users from national laboratories, universities, and industry leading to new levels of understanding about fundamental properties and processes in a wide range of systems. Also, inelastic x-ray scattering will likely be the dominant spectroscopic technique at LCLS and it is therefore an important strategic advantage to also emphasize it at SPEAR3.

In particular, XRS will widen the range of XAS on low-Z samples traditionally performed in the soft x-ray range, to systems and sample conditions where the penetration of a hard x-ray probe is essential. RIXS spectroscopy provides detailed information on the local electronic structure and spin states of, e.g., 3d transition metal compounds with hard x-rays. As compared to conventional K-edge XAS it can better isolate lowest unoccupied molecular orbital (LUMO) resonances and has less lifetime broadening along the energy transfer axis. Furthermore it provides L-edge/M-edge like information with the advantage of a hard x-ray probe. Site-selective EXAFS combines the chemical sensitivity of Kβ XES with EXAFS to provide more detailed structural information in mixed valence systems, and range-extended EXAFS will increase the spatial resolution by overcoming the k-range limits from neighboring absorption edges. XES contains chemical and structural information complementary to XAS, in particular with regards to the oxidation state, spin state and the type of ligand.

4.3.D. Facilities for Time-Dependent Studies

We propose the development of general facilities for performing time-resolved experiments in both the hard and soft x-ray range at SPEAR3, probing both non-equilibrium and equilibrium dynamics in materials, on time-scales extending from picoseconds to seconds. Under present operating conditions the time structure of SPEAR3 consists of 39 ps FWHM pulses, separated by 2.1 ns. We have recently successfully operated SPEAR3 with a low momentum compaction lattice that reduces the bunch length. We can operate with 280 bunches as follows:

15 ps FWHM with 0.27 nC per bunch or 100 mA total current,

9 ps FWHM with 0.05 nC per bunch or 17 mA total current,

6 ps FWHM with 0.003 nC per bunch or 1 mA total current.

The beam emittance increases from 18 to 40 nm-rad in the short bunch lattice. This SPEAR3 capability is available without the addition of complex and expensive components.
The unifying idea of our proposal is the combination of small x-ray spots with time-resolved x-ray scattering and absorption techniques. The focused x-ray beams may be used to probe dynamics on length-scales set by the x-ray spot size. The full or almost full use of the repetition rate of the ring will be used by use of a state-of-the-art high-rep rate, ultrafast laser system to probe equilibrium and non-equilibrium dynamics in condensed matter.

In the *hard x-ray range*, pump-probe experiments will be carried out at beamline 6-2, an insertion device beamline with a 54 pole wiggler at SPEAR3. A Kirkpatrick-Baez (KB) focusing system produces an adjustable spot size from 1-10 µm with a working distance of ~6 cm. Many of the experiments described below probe time-resolved changes in the structure factor *S(q,t)* in disordered systems, for which the diffraction peaks are significantly broadened compared to perfect crystals. The required energy resolution is thus significantly reduced, allowing one to use a pair of multilayer mirrors as a monochromator, with ~ 2 orders of magnitude increase in flux compared to a silicon (111) monochromator.

We estimate that at 500 mA, a flux on order 5 x 10^{12} photons/second can be produced in a 10 micron diameter spot at the 476 MHz repetition rate of the ring. A femtosecond long cavity Ti:Sapphire oscillator will be used to produce high energy (~100 nJ/pulse) pulses at 800 nm at 10 MHz repetition rate, the 47th subharmonic of the 476 MHz radio frequency which drives the

SPEAR3 ring. By focusing to a 10 micron spot size, one reaches a fluence of 100 mJ/cm^2 (~1.5 TW/cm^2), which is of order the single shot damage threshold of most materials. For many experiments, significantly less energy will be required. This laser will also be used in some of the soft x-ray experiments described below.

At 10 MHz with no increase in the current/pulse, one would have ~ 10^{11} useable photons/second incident on the sample and overlapped with a femtosecond laser pulse, making weakly scattering, disordered systems easily within reach. The use of microfocused x-rays provides another important improvement from typical time-resolved x-ray experiments in that gated detectors or high speed x-ray choppers need not be used, since one effectively makes use of every pulse provided by the synchrotron. This allows one to use large area detectors without gating, with important gains in quantum efficiency and active area of the detectors.

The *soft x-ray* experiments will be implemented on BL13 and use an x-ray zone plate to produce an x-ray spot as small as 100 nm at a focal distance of 20 mm. Because we intend to study the dynamics on submicron length scales we need to be able to position the x-ray spot onto the area of interest. For this purpose the sample can be moved perpendicular to the x-ray beam using two different piezo elements. Furthermore we want to be able to vary the size of the probing area between 0.1µm and several micrometers. This can be achieved by changing the distance between the sample and the zone plate along the x-ray beam by only a few hundred micrometer using additional piezo elements as well. The x-ray absorption signal can be measured by either detecting the secondary electron yield or the intensity that is transmitted through the sample using a fast photodiode. The detector signal will then be read by suitable electronics that have already been developed at SSRL and were successfully used in a series of experiments at the ALS. These electronics comprise of a field programmable gate array (FPGA) and a fast serializer/deserializer that allows ultrafast counting (typically 500 MHz) of the incoming x-ray pulses. At the same time one can generate fast pump pulses that are synchronized to the incoming x-ray pulses to excite the sample via field or current pulses. A femtosecond optical pulse from the laser may also be coupled into the sample.

4.3.E. Other Facilities

Proposals for the funding of facilities A-D, identified above, have been submitted to funding agencies. In addition, SSRL is presently considering other facilities which will serve new user groups or add to the existing generic x-ray facilities.

SSRL will also take advantage of suitable proposals by user groups to implement participating research team (PRT) beam lines. Such beam lines are based on a *quid pro quo* arrangement that are worked out between the teams and SSRL management and approved by the SSRL SAC.

4.3.F. Accelerator Improvements

A primary priority for the SSRL Accelerator Systems Department (ASD), beyond providing reliable accelerator operation for users, is to improve accelerator performance with the aim of enhancing beam quality for users. In addition to the immediate plan to implement top-off injection (Section 3.3), the ASD is pursuing ongoing programs to increase beam stability, improve accelerator diagnostics and develop more accurate beam modeling and lattice control codes for the nominal SPEAR3 operating configuration. New accelerator configurations and technologies are also being investigated that would enable timing mode, short-bunch and fast polarization switching modes of operation.

As is the case for most synchrotron light sources, the goal for beam orbit stability is <10% of the photon beam's transverse rms dimensions. In the nominal SPEAR3 lattice configuration, this level of stability translates to the order of 20 µm horizontally and a few microns vertically. Requirements for longitudinal (time-of-arrival and energy oscillations) bunch stability depend on the parameter of interest: < 10% (<1.7 ps) for time-of-arrival experiments, and < ~0.5% (0.1 ps) to preserve the line width of a 7th undulator harmonic, for example. SSRL has formed a "noise abatement team", comprised of accelerator and beam line experts, to continually assess beam stability issues and to identify improvement plans to reach stability goals. The team works to identify the sources of orbit motion that persist in spite of the 100-Hz orbit feedback system, which maintains stability to a fraction of a micron as measured with monitors used for feedback, but not as measured with independent beam line detectors. The source of longitudinal oscillations, now barely within the time-of-arrival limit but not within the undulator line width limit, has been identified as being induced by rf klystron voltage ripple, and a feedback loop is now being implemented to solve this problem. Other longer range plans are being formulated, including improving the temperature stability of beam line optical components, photon monitors and the entire storage ring itself, as well as implementing bunch-by-bunch transverse feedback systems to reduce the disturbed orbit transient time during top-off injection and other potential transverse instabilities that may arise under different operating configurations. Improvements in beam instrumentation are underway, including installing high-resolution, turn-by-turn electron position monitor processors and implementing synchrotron light profile monitors capable of resolving small vertical beam sizes and picosecond bunch lengths.

Essential to achieving optimal accelerator operation and deriving new operating configurations are the beam and lattice simulation and characterization codes used by accelerator physicists. The storage ring accelerator physics community is very active in developing these codes to include significant non-linear effects, vacuum chamber impedances and rf structures and more accurate representations of insertion device fields, all of which contribute to complex beam dynamical behavior that determine lifetime and dimensional properties. SSRL physicists continue to make a significant contribution to these developments by expanding the LOCO linear optics characterization and AT accelerator toolbox and tracking programs. The use of these programs, along with other modern modeling and beam-based machine characterization methods, such as frequency map analysis and turn-turn beam position analyses, have enabled not only the optimal tuning of the nominal SPEAR3 lattice, but also the successful implementation of the new double-waist chicane lattice (used for the small-gap, in-vacuum undulator for BL 12), improved specifications for insertion device magnetic field quality and the investigation and development of potential new operating modes, such as those having short bunch lengths.

In pursuit of short bunch operation for SPEAR3, which is of significant interest for SSRL, both equilibrium and non-equilibrium implementations are being considered. One equilibrium scheme that has already been demonstrated is the low momentum compaction (or low-alpha) lattice discussed in section D above. Orbit stability in this lattice is much more sensitive to small magnetic and rf perturbations, so work will continue to improve the low-current operation of the orbit and longitudinal rf feedback systems for this mode. Other equilibrium short bunch schemes are being considered, including using crab cavities to create localized short bunches in the ring. The beam dynamics of one non-equilibrium method is being investigated where a sub-picosecond beam is injected for a limited number of turns around the ring and then discarded before the bunch length becomes excessive.

The ASD works with SLAC accelerator research and analysis groups to address SPEAR3 performance issues and improvement possibilities. Many vacuum chamber impedance analyses are done in collaboration with the Advanced Computation Department, while the Beam Physics Department is consulted for many lattice development and beam dynamics issues. A potentially fruitful dialogue has been initiated with the Advanced Technology Research Department (ATRD), which specializes in high-power and novel rf device development, to assess the possibility of building a large aperture, pulsed microwave undulator capable of switching planar and/or elliptical polarizations very quickly, from 360 Hz to >10 MHz, depending on implementation. The ATRD would also be involved with the design of rf beam manipulation devices (e.g. crab or harmonic rf cavities) as well has high-performance bunch feedback systems. These research groups will be integrally involved in conceiving and developing new operating modes and technologies for enhanced performance of SPEAR3 and its injector as well as in conceiving new ideas for future photon sources at SLAC.

4.4 Formation of a task team to plan for new photon sources at SLAC

It is the goal of SSRL to remain a state-of-the-art synchrotron radiation facility that supports a broad spectrum of users. Thus any source based on an upgrade or replacement of SPEAR3, needs to emphasize improvements in *average brightness,* in contrast to a specialized machine like LCLS that is based on *peak brightness.* A trade-off between different modes of operation may be desirable. Based on present knowledge such approaches would include:

- Complementing and/or converting of SPEAR3 to incorporate an energy recovery linac (ERL), having very low emittance, high rep rate and short bunch length,
- Developing the 2.2-km PEP-II ring facility into a new ultrabright light source,
- Developing a new compact high-charge, short bunch, high rep rate photon source using high gradient laser and/or plasma wakefield acceleration,
- Pursing new FEL technology that exploits unforeseen combinations of high-power rf, laser and novel accelerator technologies.

SSRL has formed a task force headed by Robert Hettel and Ingolf Lindau to explore possibilities for new photon source development at SLAC. The group will be comprised of photon science and accelerator experts who will formulate an initial plan by mid 2007 that would uniquely position SSRL in relation to the rest of the international light source community for performing state-of-the-art research in future years. The team will meet on a continuing basis and will advise the SSRL Director on new developments and opportunities. The SSRL Director will integrate the team's recommendations into the strategic plans of the SLAC site.

The task force will especially explore the ultilization of the PEP-II storage ring for a next generation x-ray source. Because of its large circumference of 2,200m (in comparison to APS 1,060m and NSLS-2 620m), one or both of the storage rings in the PEP tunnel could be converted to very low emittance light sources (order 0.1 nm-rad). The study group is exploring not only PEP's potential as a very high brightness conventional storage ring light source operating in a "general user mode", spanning the soft to hard x-ray spectrum (up to 100 keV), but also the possible implementation of novel x-ray sources using bypasses around the ring or possibly the second ring itself. These areas allow localized electron bunch compression and the possibility of soft x-ray FEL implementations so that x-rays of different characteristics and variable repetition rates may be delivered to different users. This concept would circumvent the development of energy recovery linacs or superconducting high-brightness electron guns required in other proposals to implement high rep-rate (100-1000 kHz) tunable soft x-ray FELs. The envisioned PEP light source operating modes include the general user mode, a pump-probe ultrafast mode having high average brightness, and a high peak brightness mode using the high rep-rate FELs. The 2-ring concept might permit simultaneous operation of the general user and specialized modes.