2005 Update For SLAC Users Annual Meeting  September 26, 2005

Glenn Waychunas, SSRLUOEC Chair

• SSRL 2004-2005 recap
• SPEAR3 Success
• Scientific Highlights
• SSRL 32nd Annual Users Meeting
• User/SSRLUOEC activism
SSRL User Operations

- User operations on 19 beam lines during this 2nd post-SPEAR3 user run (10/04 accident resulted in 4 mo. shutdown)
  - BL2-2 no longer available for user operations due to 2005 budget cuts
  - BL3 TBD
  - BL5-1/2 in commissioning phase; users operations in 2006
  - BL4 upgrade pending (2006 shutdown); back to users in 2007
    - BL4-2 has been available in the interim
  - BL7 upgrade currently underway; back to users in early 2006
- >900 on-site users during 2005 6-month run, including SPPS (average 150 users/month)
  - 680 on-site users during 5-month run in 2004 (136 users/month with staggered starts on 19 BL’s)
  - 867 on-site users during 5-month run in 2003 (173 users/month on 27 BL’s)
  - 1,023 on-site users during 8-month run in 2002 (128 users/month on 24 BL’s)
- 761 experimental starts in 2005 (average 126 starts/month)
  - 466 experimental starts in 2004 (93 starts/month)
  - 666 experimental starts in 2003 (133 starts/month)
  - 1,011 experimental starts in 2002 (126 starts/month)
- User statistics analyzed and incorporated into DOE quarterly and annual reports
## Summary of User Operations

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<tbody>
<tr>
<td>Months Operating</td>
<td>6</td>
<td>5</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td>Operating BL's</td>
<td>19</td>
<td>19</td>
<td>27</td>
<td>24</td>
</tr>
<tr>
<td>On-Site Users</td>
<td>&gt;900</td>
<td>680</td>
<td>867</td>
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<tr>
<td>Exp. Starts</td>
<td>761</td>
<td>466</td>
<td>666</td>
<td>1,011</td>
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Notes:
- 2002-Last “regular” year of user operations before shutdown for SPEAR3
- 2003-BL1-5,11-3,SPP-1 added; shutdown 3/03 for SPEAR3 installation
- 2004-Operations resumed 3/04 with 19 BL openings staggered ~ every 2 weeks
- 2005-Lost 4 months of scheduled 9-month run due to electrical accident; run extended from July 5th to Aug. 1st
- 2006 projections: 8 month run (11/28/05-7/31/06) on 23 BL’s (includes BL3-1, 5-1/2, 7-1, 7-3; ~1,000 experimental starts, ~1,200 on-site users
For the last two run periods the user breakdown by proposal discipline:

**Materials Science** 14%
**SS Physics** 5%
**Chemistry** 16%
**Polymers** 2%
**Medical Applications** 5%
**Biology/Life Science** 45%
**Earth/Environ. Sci.** 8%
**Optics/Engineering** 4%
**Instrument Develop.** 1%
### Publications as a Metric of User Productivity

- 7,008 SSRL user publications have been reported since 1974 (journal articles, books, conference proceedings, theses)
  - 176 publications reported to date in 2005
  - 410 publications in 2004
  - 433 publications in 2003
  - 432 publications in 2002
  - 465 publications in 2001
  - 440 publications in 2000
  - 380 publications in 1999
  - 344 publications in 1998
2005 User Operations

Average Demand in 2005 was ~160%
(High of ~260% on BL2-3, 9-3, 11-1, 11-2; Low of ~60% on BL1-5)

Average Rating Per Scheduled Beam Time = 1.35
(Highest Average Rating = 1; Lowest Average Rating = 2.07)
End of Run Summary feedback from Users

User groups complete End-of-Run Summary after each visit

**Overall Scientific Experience**

- Percentage of Responses

**Beam Quality**

- Percentage of Responses

* “Somewhat satisfactory” rating added when survey revised in March 2001.
SPEAR3 success

- Replaced SPEAR2 ring during 2003 shutdown
- Successful run during 2004 on reduced schedule
- Dramatic improvements in brightness, reduced emittance
- Recently tested successfully at full design current of 500 ma

<table>
<thead>
<tr>
<th>Table 1. Parameters for SPEAR 2 and SPEAR 3.</th>
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<tbody>
<tr>
<td>Parameter</td>
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<tr>
<td>Energy</td>
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<tr>
<td>Current</td>
</tr>
<tr>
<td>Emittance (w/ID)</td>
</tr>
<tr>
<td>RF frequency</td>
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<tr>
<td>RF gap voltage</td>
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<tr>
<td>Lifetime @ Imax</td>
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<tr>
<td>Critical energy</td>
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<tr>
<td>Tunes (x,y,s)</td>
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<tr>
<td>e- σ (x,y,s) - ID</td>
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<tr>
<td>e- σ (x,y,s)-dipole</td>
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<td>Injection energy</td>
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<tr>
<th>Table 2. Relative increase in photon flux and brightness for SPEAR 3.</th>
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<td>Beam Line</td>
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<tr>
<td>bend</td>
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<tr>
<td>BL4/7 ID</td>
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<td>BL9 ID</td>
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SPEAR3 Beam Fill and Top-Off Options

a. 100 mA (vacuum quality = 5-6 A-h, with IDs)

b. 500 mA (vacuum quality = 7 A-h, with IDs)
Examples of Synchrotron Science

The molecular biology of Anthrax infection

Initial phase of infection:
- Anthrax Toxin binds to cell receptor
- Toxin undergoes rearrangement
- Rearranged toxin then binds with other Anthrax toxin enzymes
- These enzymes enter and kill victim’s cell

By understanding the chemical details of the toxin-cell binding, drugs to treat Anthrax or produce immunity are possible.

Study of this mechanism also reveals a possible Cancer treatment
- The Anthrax toxic unit also binds to a tumor marker which is common on cancer cells
- The toxin might be tailored to specifically interrupt cancer mechanisms

Examples of Synchrotron Science

Investigations to Identify the Soluble, Non-pertechnetate Species in the High-level Nuclear Waste at the Hanford Site

Wayne W. Lukens¹, David K. Shuh¹, Norman C. Schroeder², Kenneth R. Ashley³

¹Lawrence Berkeley National Laboratory, Berkeley, CA
²Los Alamos National Laboratory, Los Alamos, NM
³Texas A&M University-Commerce, Commerce, TX

Tc is an abundant fission product that poses a number of challenges for the safe disposal/encapsulation of high-level nuclear waste.

Studies at SSRL determined the structure of Tc complexes stable at high pH, and indicate the importance of non-pertechnetate complexes such as the carbonyl and nitroyl Tc(I) variants.
When a blood vessel is injured, a repair mechanism is initiated through the formation of a hemostatic plug that seals the wound. This life saving process becomes life threatening when clots form inside functional vessels leading to pathological thrombosis. Arrest of bleeding is achieved via platelet adhesion and thrombin-related fibrin clotting at the injury site. In order for the platelets to stick to the injured tissue and each other, they need to be activated. In addition to causing fibrin clotting, the protease thrombin plays a crucial role in activating platelets, and its action is tightly regulated due to its procoagulant and anticoagulant activities. Hence the molecular details of the action of thrombin with platelets are required for a proper understanding of the clotting process.
Examples of Synchrotron Science

The Structure of the First Coordination Shell in Water

Ph. Wernet¹, D. Nordland², U. Bergmann³, M. Cavalleri², M. Odelius², H. Ogasawara⁴, L. Å. Naslund⁴, T. K. Hirsch², L. Ojamae⁵, P. Glatzel⁷, L. G. M. Pettersson², A. Nilsson⁴*

¹ Stanford Synchrotron Radiation Laboratory, Post Office Box 20450, Stanford, CA 94309, USA; Present address: BESSY, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany.
² FYSIKUM, Stockholm University, AlbaNova, S-106 91 Stockholm, Sweden.
³ Stanford Synchrotron Radiation Laboratory, Post Office Box 20450, Stanford, CA 94309, USA.
⁴ Stanford Synchrotron Radiation Laboratory, Post Office Box 20450, Stanford, CA 94309, USA; FYSIKUM, Stockholm University, AlbaNova, S-106 91 Stockholm, Sweden.
⁵ Department of Physical Chemistry, Stockholm University, S-106 91 Stockholm, Sweden.
⁶ Department of Chemistry, Linköping University, S-58183 Linköping, Sweden.
⁷ Department of Inorganic Chemistry and Catalysis, Debye Institute, Utrecht University, 3584 CA Utrecht, Netherlands.

Studies of water structure using X-ray absorption spectroscopy and X-ray Raman scattering have allowed a new interpretation of liquid water molecular structure based on measurement of the electronic (Molecular orbital) structure.

Water is found to differ essentially from ice (with tetrahedral neighbors), instead favoring chain or ring associations.

ZnS nanoparticles (3 nm diameter) are found to have disordered surfaces that propagate strain and atomic displacements into the core of the particle. The strain incorporates a radial distortion, random (thermal) displacements, and a kind of mosaic strain modeled by a SRO parameter. The high degree of strain accompanies a higher Debye temperature than for bulk ZnS. Analysis was done via PDF (x-ray scattering) and varied temperature EXAFS studies.

SSRL Users Organization (SSRLUO)

• Acts as liaison between Users and SSRL administration
• Plans, Organizes and Hosts an annual User’s Meeting
• Sponsors and presents Annual Farrel W.Lytle and W.E. Spicer awards
• Holds Graduate Student poster competition at meeting
• Elects members to serve on the executive committee to carry out the business of the SSRLUO

SSRLUO-EC

• SSRLUO-EC is the (voluntary) formal organizational unit of the SSRL Users Organization
• Members serve at least 2-year terms
• Chair and vice-chair elected by the SSRLUO-EC
• Chair serves for 1 year; vice-chair rotates into the chair position the following year; former chair serves as ex-officio for 1 year
# SSRLUO-EC 2004-5 Members

13 scientists, including 2 students, elected by the SSRL users

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution and Department</th>
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<tbody>
<tr>
<td>Glenn Waychunas</td>
<td>LBNL, Environmental Sciences</td>
</tr>
<tr>
<td>Joy Andrews</td>
<td>CSU Hayward, Materials Chemistry</td>
</tr>
<tr>
<td>Ben Bostwick</td>
<td>Dartmouth College, Environmental Sciences</td>
</tr>
<tr>
<td>Juana Acrivos</td>
<td>San Jose State Univ., Materials Chemistry</td>
</tr>
<tr>
<td>Alex Bell</td>
<td>UC Berkeley, Materials Chemistry</td>
</tr>
<tr>
<td>Linda Brinen</td>
<td>UCSF, Macromolecular Crystallography</td>
</tr>
<tr>
<td>Michael Brzustowicz</td>
<td>Stanford Univ. (School of Medicine), Structural Molecular Biology</td>
</tr>
<tr>
<td>Lisa Downward</td>
<td>UC Santa Cruz, Graduate Student</td>
</tr>
<tr>
<td>Richard Lee</td>
<td>Physics and Advanced Technologies (LLNL), LCLS</td>
</tr>
<tr>
<td>Kate Newberry</td>
<td>Oregon Health Sciences Univ., Macromolecular Crystallography</td>
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<tr>
<td>Joseph Noel</td>
<td>Salk Institute, Macromolecular Crystallography</td>
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<tr>
<td>William Schlotter</td>
<td>Stanford Univ., Graduate Student</td>
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<tr>
<td>Timothy Stemmler</td>
<td>Wayne State Univ., Structural Molecular Biology</td>
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<tr>
<td>Cathy Knotts</td>
<td>User Research Administration, SSRL, SLAC</td>
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<td><strong>Cathy Knotts (SSRL Liaison)</strong></td>
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Highlights of 31st Annual Users Meeting

Co-chairs: Michael Toney and Glenn Waychunas
Organizing committee: Cathy Knotts, Lisa Dunn, Michelle Steger and Jacqueline Robleto, co-chairs

• Symposium honoring contributions of W.E. Spicer
• First W.E. Spicer Young Investigator Award to N. Peter Armitage
• Lytle Award to W. Hal Tomkins
• Young Investigators Symposium
• 35 Posters Presented
Winners: Eric Dugans (UCB), Rinku Jain (OSU), Aaron Slowey (SU)
• Over 350 Attendees (largest total attendance)
• Other Sessions on Spectroscopy, Changing times at SSRL, Scattering, Diffraction, and Tomography, SSRL Facilities Reports

32nd Annual Users Meeting in three weeks
Examples of Recent SSRLUO-EC Activities

Coordinating activities and communications

- As a follow-up to meeting with Drs. Raymond Orbach and James Decker in 2002, SSRLUO-EC has started to work with SLUO
- One outcome is the Public Speakers Program (initiated last year by Uwe Bergman). This is an important outreach tool for the local community.
- Letter of appreciation signed by all four DOE synchrotron user organization chairs sent to DOE

User activism

- Trip to Washington DC to meet with staff from various committees in planning, particularly OMB and congress appropriations committees. Timing chosen to support synchrotron funding in 2006 (markup) and 2007 (planning) budgets.
- Meet with local and other congressional representatives affecting synchrotron source funding.
- Encourage other users to contact their state representatives
- Coalescence of all DOE synchrotron and neutron Users group user activism being planned