Light Sources Based on Linear Accelerators

Linac-driven Light Sources - Toward the 4th Generation



Single pass linear colliders Eliminating bending magnets makes it possible to reach very high energy (no synchrotron radiation losses)

Single pass linear light sources Free electron lasers (FELs) Energy recovery linacs (ERLs)

Eliminating bending magnets makes it possible to produce very low emittance electron & photon beams and very short (fs) pulses



From AMO2010 report

Synchrotron radiation from Storage Rings is a very powerful tool for the study of material on the atomic and molecular scale

Although the pulses of light from storage rings, particularly from wigglers and undulators, are very intense, their pulse length is measured in tens of picoseconds.

To study processes on a faster time scale, typical of atomic and molecular processes, an intense source with a shorter pulse duration is needed.

The Free-Electron Laser provides this. Femtosecond pulse durations with >10¹² photons per pulse Brightness and Pulse Length in Electron-based X-ray generation

- X-ray brightness determined by electron beam brightness
- X-ray pulse length determined by electron beam pulse length

Storage ring ("conventional synchrotron radiation") Emittance and bunch length are result of an equilibrium Typical values: 2-100 nm-rad, 50 psec

Linac (source for x-ray FEL or ERL)

Normalized emittance is determined by electron gun Bunch length is determined by electron compression Possible values: 0.03 nm rad, 100 fs or shorter

Linac beam can be much brighter and pulses much shorter! – at cost of "jitter"- and provides necessary characteristics for ERLs or x-ray FEL generation

Frontier tools for x-ray science: ultrafast science



10 11 12 13 14 15 16 17 18 18



Emittance and Pulse Length in Rings & Linacs

Rings; Emission of SR in bending magnets results in

- Electron energy spread which increases bunch length *Typical bunch lengths are ~50 picoseconds*
- Betatron oscillations which cause emittance growth

Emittance scales as $\mathcal{E} \sim E^2 \theta^3$ (θ is the angle of bending in each bend magnet) Third generation rings have $\mathcal{E} \sim 5 \times 10^{-9} m$

Linacs: No bends, hence no SR emission (except compressors)
•Electron emittance determined mainly by source (gun) emittance
•Emittance scales with (electron energy)⁻¹ ε~1/E reach diffraction-limited emittance, ε=λ/4π=10⁻¹¹m for λ~1.5Å
•Bunches can be compressed to sub-picosecond levels

*Emittance is the product of beam size and divergence; meters x radians

Origin of Emittance in Rings

- Quantum nature of photon emission → energy spread in electron beam
- Different energies are dispersed in bending magnets → different orbits for different energies
- Emission of a photon by electron on its proper orbit → sudden shift in equilibrium orbit. Since electron position does not change during photon emission, the electron begins to execute betatron oscillations about suddenly displaced equilibrium orbit → larger beam size/emittance



Emittance in a Storage Ring



Approaches to Reducing Emittance in Storage Rings

- Reduce emission of radiation in bending magnets → lower electron energy and weaker field → <u>larger circumference</u> (CESR, Petra, PEP, Tristan) for a given energy. Radiated Energy ~ E²B²
- 2. Reduce length of bending magnet to reduce separation of orbits of electrons with different energies. *i.e.; reduce dispersion*
- ⇒ Above considerations lead to designs with small angular deflections in each bending magnet. Quadrupoles between bends refocus the beam before it gets too large.

Emittance $\mathcal{E} \sim E^2 \Theta^3$ E = electron energy Θ = angular deflection in each bending magnet

Importance of low emittance in a light source first emphasized by R. Chasman and K. Green at BNL in 1976.



For a Gaussian Distribution

 $\varepsilon_{X\gamma} = \sigma_{X\gamma} \bullet \sigma_{X'\gamma} \ge \lambda/4\pi =$ Minimum Photon Beam Emittance

•	I	Examples	S	
hv (eV)	10	100	1,000	10,000
λ (nm)	124	12.4	1.24	0.124
ε (nm-rad)	10	⊢ 1	0.1	0.01
I	Present	3 rd Gene	eration Ri	ngs

Circumference of Storage Rings

Tantalus	SPEAR	NSLSII	APS	SPring8	PEP/PETRA	LHC
10m	230m	800m	1000m	1450m	2,200m	27,000m

Origin of Emittance in Linacs

- Radiation effects not important
- Emittance determined by the electron source the gun
- Emittance decreases with energy $\varepsilon \sim \gamma^{-1}$
- Can achieve lowest emittance in high-energy linacs equipped with a high-brightness electron source (*photocathode RF gun*)

At Cathode



After Acceleration in Linac



Compared to storage ring beams, electron beams from a linac can have

- Lower emittance
- •Higher peak current

Shorter bunch length

This makes linacs better drivers for Energy Recovery Linacs and Free-Electron Lasers.

The beam in a storage ring circulates for many turns. Its properties are determined by radiation effects and the magnet lattice. The properties of the electron source are largely irrelevant once the beam is stored in the ring.

The beam in a linac is used only once; it is a single pass device. Its properties are determined by the electron source, the gun. Radiation effects are very small in a linac since there are no bending magnets.

Bright electron beams from linacs open a path for the Energy Recovery LINAC (ERL)

- Very short and coherent pulses
- Time-averaged brilliance like 3rd generation sources
- Upgrade path could be minimally disruptive





Figure 1: Jefferson Lab 1 kW IR FEL. The machine is shown in the facility vault.



Figure 1: 35 MeV ERLP layout at Daresbury

Cornell Design for an Energy Recovery Linac

http://www.lepp.cornell.edu/Research/AP/ERL/rsrc/LEPP/Research/AP/ERL/WebHome/05cornell.pdf



Layout of the existing CESR ring (6) and the ERL upgrade

Electrons from an injector that is optimized for very narrow and short electron pulses (1) would be accelerated to the right in a first linear accelerator or linac (2). A return loop (3) would send them into a second linac which is located in the same straight tunnel (4) and accelerates to the final high energy. An arc (5) injects the electrons into the already existing CESR ring (6) where they travel clockwise until another arc (7) injects them back into the first linac, where they are decelerated to half their energy. The return loop leads the electrons to the second linac section where they are decelerated back to their low injection energy with which they are finally dumped (8).

Very bright electron beams from linacs open the path to short wavelength Free-Electron Lasers

Interaction of a *bright electron beam* with a strong *optical field* in an *undulator magnet* results in a *density modulation* of the electron bunch at the *optical wavelength* \rightarrow *coherent emission*

i.e.; proportional to the square of the number of electrons (N²) within an optical wavelength rather than linearly with N as in spontaneous synchrotron radiation.

Linac-driven Light Sources - Toward the 4th Generation

Conventional Undulator -Spontaneous Emission



The X-ray Laser operates by grouping electrons so that they work together to produce many more X-rays than each electron alone.

One thousand electrons packed closely together can radiate **one million** times more than a single electron!!

Bunched electrons radiate coherently







END

Linac-driven Light Sources - Toward the 4th Generation



XFELs coming soon

Physics Today, May 2005

X-Ray Free-Electron Laser Projected Parameters							
	LCLS (US)	DESY XFEL (Europe)	SCSS (Japan)				
Pulse duration	<230 fs	100 fs	80 fs				
Wavelength	1–64 Å	1–15 Å	1–50 Å				
Repetition rate	120 Hz	10 Hz	60 Hz				
Electron bunches per pulse	1	≤3000	1				
Electron beam energy	4-14 GeV	≤20 GeV	≤8 GeV				
Photons per pulse (×1012)	1.2 (at 1.5 Å)	1.2 (at 1 Å)	0.76 (at 1 Å)				
Linac length	1 km	2 km	350 m				
Estimated cost*	\$379 million	\$1 billion	\$330 million				
Estimated start date	2009	2012	2010				
*Estimates include varying amounts of instrumentation and different methods of accounting.							







•SLAC-PUB-611



Program developed by international team of scientists working with accelerator and laser physics communities

"the beginning.... not the end"



Femtochemistry

Nanoscale Dynamics in Condensed matter

Atomic Physics

Plasma and Warm Dense Matter

Structural Studies on Single Particles and Biomolecules

FEL Science/Technology

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X-FEL Pulses are Extremely Bright







Linac Coherent Light Source at SLAC X-FEL based on last 1-km of existing 3-km linac 1.5-15 Å Injector (35°) (14-4.3 GeV) at 2-km point Existing 1/3 Linac (1 km) (with modifications) New e⁻ Transfer Line (340 m) Undulator (130 m **Iransport** Line (200 m) **Near Experiment Hall** Argonne Far Experiment



LCLS Undulator Hall

Experimental Halls and Operations Schedules







LCLS Accelerator and Compressor Schematic



J. Arthur: FEL Intro

4 July

2006

Electron bunch compression



Acceler Center

SSRL



SPring-8 Angstrom Compact free electron Laser (**SACLA**) First lasing, June 7, 2011





Niobium Accelerating covity





European X-FEL Components




Construction of Injector Vault on DESY site; April 4, 2011



The second tunnel section on 02 December 2010 X-Ray Diffraction from Single Molecules – J. Hajdu, Uppsala Univ.

A bright idea:

Use ultra-short, intense x-ray pulse to produce scattering pattern before molecule explodes



SAMPLE INJECTOR

THEORY predicts that *intense* and *short* X-ray pulses may allow high resolution imaging of single particles and biomolecules

Neutze, Wouts, van der Spoel, Weckert, Hajdu *Nature* 406, 752-757 (2000) detectors

X-fel pulse



Concept: Capture an image before the sample has time to respond (explode)

3D reconstruction from many views





X-ray diffraction pattern of a single Mimivirus particle imaged at the LCLS. In this study, the X-ray pulse lasted a millionth of a billionth of a second and heated the virus to 100,000 degrees Celsius, but not before this image was obtained. (Image courtesy Tomas Ekeberg, Uppsala University.)



<u>SAMPLE</u>

Micron sized features On Silicon Nitride film

Single 25 femtosecond pulse; 10¹² X-rays (*FLASH* FEL at DESY)

DIFFRACTION

PATTERN

<u>RECONSTRUCTED</u> <u>IMAGE</u>

Data recorded before sample was destroyed (temperature 60,000K)

Femtosecond diffractive imaging with a soft-X-ray free-electron laser

Henry N. Chapman, Anton Barty, Michael J. Bogan, Sébastien Boutet, Matthias Frank, Stefan P. Hau-Riege, Stefano Marchesini, Bruce W. Woods, Sa a Bajt, W. Henry Benner, Richard A. London, Elke Plönjes, Marion Kuhlmann, Rolf Treusch, Stefan Düsterer, Thomas Tschentscher, Jochen R. Schneider, Eberhard Spiller, Thomas Möller, Christoph Bostedt, Matthias Hoener, David A. Shapiro, Keith O. Hodgson, David van der Spoel, Florian Burmeister, Magnus Bergh, Carl Caleman, Gösta Huldt, M. Marvin Seibert, Filipe R. N. C. Maia, Richard W. Lee, Abraham Szöke, Nicusor Timneanu and Janos Hajdu

Nature Physics (online): 12 November 2006

The image was obtained In a single pulse from a 2-dimensional object

10¹² photons at λ=32 nm (4x10¹³W cm⁻²)

The sample was destroyed, but the reconstructed X-ray image shows no evidence of this

Paves the way to 3-dimensional imaging of a single molecule (without crystals)

Other X-FELs with Hard X-Ray Capabilities

0.1 - 4 nm SACLA 2011 at SPring-8 X-FEL at **DESY** 0.1 - 6 nm 2015 Swiss-FEL at PSI 0.1 - 7 nm 2016 0.1 - 6nm PAL X-FEL at Pohang 2016?

Several others at longer wavelength such as

Fermi-FELat Trieste6 - 40 nm2013

FERMI – FEL, at Trieste

Layout





Abstract of Claudio's paper at 1992 Fourth Generation Workshop

We show that using existing electron gun technology and a high energy linac like the one at SLAC, it is possible to build a Free Electron Laser operating around the 4 nm water window. A modest *improvement in the gun performance would further* allow to extend the FEL to the 0.1 nm region. Such a System would produce radiation with a brightness many orders of magnitude above that of any synchrotron radiation source, existing or under construction, with laser power in the multigigawatt region and subpicosecond pulse length.



10²

7533A1

Next Generation Photocathode RF gun BNL/SLAC/UCLA



LCLS BACKGROUND

1. Workshop on the Prospects for a 1 A FEL; Sag Harbor, NY; April 22-27, 1990. J. Gallardo, R. Palmer

2. Workshop on 4th Generation Light Sources; SLAC; February 24-27, 1992. M. Cornacchia, H. Winick

3. Workshop on Scientific Applications of Short Wavelength Coherent Light Sources; October 21, 1992; SLAC; W. Spicer, J. Arthur, H. Winick

4. Workshop; Towards Short Wavelength FELs; BNL; May 21-22, 1993. I. Ben-Zvi, H. Winick

5. Workshop on Scientific Applications of Coherent X-rays; SLAC; February 12, 1994. J. Arthur, G. Materlik, H. Winick

Plus many other workshops, meetings held in Europe, Japan and the US.



LCLS PEAK AND AVERAGE PHOTON FLUX VS PHOTON ENERGY



Roman Tatchyn - SSRL - 2/11/94

Message from Burt Richter

"Claudio and Herman Winick are the real fathers of the x-ray laser. Claudio led the accelerator physics study while Herman with Artie Bienenstock and Keith Hodgson lead the effort to get the science community interested. We all know the result - an extraordinarily successful facility that has made SLAC the leader in the synchrotron radiation world, at least for a little while. I don't know what a fifth generation facility will look like, but I there is to be one, I am sure Claudio will be there."

Burton Richter

FUTURE PHOTON SOURCES

STORAGE RINGS

- Many simultaneous users Cost effective
- Extremely stable
- Well understood technology; many rings in operation

LINAC-BASED SOURCES (ERLs and FELs)

- Higher brightness and coherence
- Shorter pulses (femtosecond range)
- Few in operation

Both are needed for a bright photon science future

In Summary

• X-rays and VUV/soft x-rays have been an important probe of materials for basic and applied research for 100 years

•Synchrotron radiation from storage rings provides extremely intense x-rays, soft x-ray, and VUV beams - "big scale machines" enabling a large quantity of "individual investigator science"

•New sources (FELs, ERLs) offer major performance extensions

• We are living through a revolution in science & technology due to this immense increase in x-ray source performance over the past few decades

The future looks very "bright" indeed

"The real voyage of discovery consists not in seeking new lands, but in seeing with new eyes."

Marcel Proust

A La Recherche du Temps Perdu

Regional facilities allow a group of countries to cooperate to provide a high performance center, which is beyond the ability of a single country to fund.

e.g.; ESRF for technologically advanced countries in Europe SESAME for developing countries in the Middle East

WHY NOT AFRICA?

Physics Today, October 2003; page 32 Alexander Animalu, past president of the Nigerian Academy of Science and chairman of the Institute for Basic Research in Abuja, Nigeria,

"Given Nigeria's bloated foreign debt, high rate of inflation, mass unemployment, fuel crisis, collapse of the health and educational sectors, deterioration of the infrastructure of roads, epileptic electric power supply, religious riots, ethnic militia, and insecurity of life and property, the only hope of tackling this myriad of problems is by focusing on science- and technologydriven socioeconomic initiatives."

APPLICATIONS

Some uses of Synchrotrons

- Structural molecular biology
- Molecular environmental science
- Surface and interface science
- Nano mechanical devices
- X-ray imaging
- Archaeological microanalysis
- Material characterization
- Medical applications

Applications

Materials Research

Basic understanding of semiconductors, metals, superconductors, alloys, elementary excitations, electronic structure, phase equilibrium, actinide chemistry, . . .

Photoelectron Spectroscopy, EXAFS, Small angle scattering, powder diffraction, . . .

Surface Science

Structure of clean surfaces, ultra-thin films, chemisorption complexes, interfacial junctions, dynamic and kinetic properties of surfaces, growth modes of thin films, . . .

UV Photoemission Spectroscopy (UPS) (Angle-resolved, spin resolved)

Polymers

Structure-property relationships Small Angle Scattering (SAS)

Applications (continued)

Atomic, Optical, Molecular Physics and Chemistry

Vibration/rotation spectroscopy Infrared microspectroscopy Chemical dynamics

Molecular Environmental Science

Study of environmental contaminants

•molecular structure, composition, oxidation state, reaction mechanisms

•stability, toxicity, mobility, bioavailability, SPECIATION

Geosciences

Mineral interfaces, compositional variations and coordination chemistry of materials at high temperature and pressure in the earth's crust, amorphous geological materials, mineral phases and phase transitions at high temperature and pressure, . . .

EXAFS, XANES, IR Spectroscopy; Laser-heated diamond anvil cells

Microscopy

IR, Soft x-ray, Hard x-ray

Applications (continued)

Structural Molecular Biology (Macromolecular crystallography)

- Determination of the 3-dimensional structure of proteins
- Elucidating biological pathways
- Drug design

MAD technique makes use of tunability of synchrotron radiation

<u>Sequencing of the human genome</u> has led to the need to understand the structure and function of tens of thousands of proteins

Industrial Utilization - Enabling Basic and Applied Research

• SSRL serves the industrial research community for basic and applied research (currently 41 U.S. companies)

11 % of all users on active proposals are from industry

- 15% of all active proposals involve an industry collaborator
- Simple user agreement and provisions for proprietary research
- Examples of technological areas and companies:

Semiconductor Processes and Fabrication

AMD, Applied Materials, Balazs, DEC/Compac, Hewlett-Packard, Intel, Motorola, National Semiconductor

Catalysis

Air Products, Chevron, Exxon, The EXAFS Company,

Union Carbide

Pharmaceuticals and Drug Discovery

Agouron Pharmaceuticals, Berlex Biosciences, Bristol-Myers

Squibb, Genencor, Genentech

Materials Properties

Dupont, Exxon, Edge Analytical, IBM

Detector and Instrumentation Development

Adelphi Technology, Hirsch Scientific, Ovonics

Environmental Sciences

Boeing, Babcock & Wilcox (Hanford)

Medical Applications

Orthologics, X-ray Instrumentation Associates





Electronic Structure and Bonding - where are the electrons -

Magnetic Structure and Properties - where are the spins-















J. Arthur: FEL Intro

4 July 2006

Stanford Linear Accelerator Center



Figure 1.3.1 User profile by discipline of experiments and total number of users for the four DOE synchrotrons (ALS, APS, NSLS, SSRL). This shows the strong increase in the percentage of users in the life sciences as well as the dramatic growth in total number of users. Current projections are that the total number of users will grow to $\sim 11,000$ annually in coming years.

Materials Science



Visualizing magnetic bits on a computer hard drive



Using SR to learn how high temperature superconductors work



Using SR to make miniature mechanical and electromechanical devices



Understanding how debris causes damage to aircraft turbines



Chemistry and Biology



Measuring very low levels of mercury in fish and determining its chemical form

Cholera toxin attacking a gut cell



Studying Anthrax Toxin components to develop treatment in the advanced stages of infection



Examples of Synchrotron Science: X-Rays Illuminate Ancient Secrets

Archimedes' exceptionally advanced ideas have been lost and found several times throughout the ages. Now scientists are employing modern technology, including x-ray fluorescence, to completely read the Archimedes Palimpsest, the only source for at least two previously unknown treatises.

(Images provided by Will Noel, The Walters Art Museum)



Intensity of Pb x-ray fluorescence from a standard hair (SN-1) with 6 ppm of lead compared to that of a hair from Beethoven (LVB) as determined at APS.



X-ray fluorescence imaging ~ revealed the hidden text. This x-ray image shows the lower left corner of the page. A photograph of one page of the Archimedes Palimpsest.
Visible and UV light cannot see Archimedes' text under the gold painting done by a 20th Century forger.



Synchrotron studies at the Advanced Photon Source reveal massive amounts of lead in bone fragments from skull of Beethoven.

These findings confirm studies of Beethoven hair samples.

Researchers believe this confirms lead poisoning as cause of composer's chronic illness.
The Archimedes Palimpsest











e sideet surviving copy of important matisenatical works of Archistoles was sold at ascents in New York.

Archimedes Text Sold for \$2 Million

A reported pledge

not to limit access

to an ancient

manuscript.

By MALCOLM W. SHOWNE

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Page 81R of the Archimedes Palimpsest



Schematic Experimental Setup



Uwe Bergmann; (SSRL) Stanford Synchrotron Radiation Laboratory

X-ray Imaging of page 81R

normal view →

Fe x-ray map





Image taken by the Rochester Institute of Technology and the Johns Hopkins University. Copyright resides with the owner of the Archimedes Palimpsest.

X-ray Imaging of page 81R



X-ray Imaging of page 81R





Determining the Structure of Complex Biological Molecules by Xray Diffraction



Diffraction Process

Diffraction Pattern from NSLS



RNA Polymerase – the structure that enables the code for each protein to be used to make each protein. (Roger Kornberg et al, Stanford)

Geoscience & Environmental Science

Reactive Barrier Concept - bone ash



Scientific understanding leads to strategies for containment of toxic & radioactive waste that threatens water supplies

Concept studied at SSRL



A giant underground filter is removing uranium contamination in an aquifer in Utah EXAFS = Extended X-ray Absorption Fine Structure



Wavenumber of photoelectrons:

$$k = \sqrt{\frac{2m_e}{\hbar^2} \cdot (E - E_0)}$$

Advantages:

- Type of central atom can be selected
- Neighboring atoms can be identified
- Especially useful for dilute systems <u>Samples</u>:
- Crystalline and amorphous materials
- Surfaces
- Liquids
- Molecular gases

Coster and Veldkamp, Z. Phys. 70, 306 (1931). See also <u>X-Rays in Theory and Experiment</u> (1935), by Compton and Allison, p. 663.





EXAFS PIONEERS

Ed Stern, Dale Sayers, Farrel Lytle

Courtesy of Corwin Booth







As and Se X-Ray Absorption Edges in c-CuAsSe₂: Original Data.

Sally Hunter; SSRL, ~1975



R. Frahm Düsseldorf

Absorption spectrum of Ni metal



Exact edge position

Near edge structure (XANES) Extended structure (EXAFS)

- => Valence state of the absorbing atoms
- => Bond angles
- => Atomic distances
- => Coordination numbers
- => Identification of neighboring atoms



Fig. 7; EXAFS spectrum of Cr (VI) and Cr (III) illustrating the ability to *identify oxidation states*

Molecular Environmental Science and Synchrotron Light Sources

Who cares about the distances between atoms?

Just about everyone should, including your next door neighbor, because such distances define molecular structure which in turn defines function or properties in natural materials, including those occurring in the environment and in living cells. The molecular form or speciation of environmental contaminants, such as chromium, arsenic, lead, uranium, or plutonium, determines their toxicity and availability to organisms.

Molecular Environmental Science

• A new multidisciplinary field that has evolved over the past ten years in response to the growing need to understand chemical and biological processes affecting environmental contaminants.

• Main objective is to provide information on the types, spatial distribution, and reactivity of contaminant species.

Synchrotron Light Sources

Now play a very important role in environmental science because the extremely intense x-rays from these sources are needed to characterize the chemical speciation and physical distributions of environmental contaminants at very low concentration levels in highly complex materials.



The movie Erin Brockovich was about chromium in water; was it trivalent (no problem) or hexavalent (deadly) chromium? Synchrotron radiation answers questions like this with ease.





MOLECULAR ENVIRONMENTAL SCIENCE (MES)

Objective: Provide information on natural and man-made waste forms.

- Chemical & Physical Forms (Speciation).
- Spatial Distribution.
- Reactivity.

Fundamental understanding of the complex molecular-scale environmental processes, both chemical& biological, that affect the stability, transformations, mobility and toxicity of contaminant species.

Speciation of Contaminants



Fig. 6; Speciation of contaminants & the role of synchrotron radiation

MES User Research at SSRL

- 291 Users/Collaborators
- 87 Active proposals with significant MES component.
- 1994, 8-hr shifts were assigned for MES proposals in 2002.



Time-dependent reduction of selenium(VI) in the presence of green rust (Fe(II,III)oxide) at pH6.8. Below: STXM image of green rust. Myneni, Tokunaga, and Brown, Science 278 (1997) 1106.



Examples of MES Proposals.

- Chemistry & structure of actinide colloids in groundwater, P. Allen, LLNL.
- Radiochemistry of plutonium at the Waste Isolation Pilot Plant, *P. Hartmann, LANL*.
- Metal coordination in marine microalgae, F. Morel, Princeton.
- Speciation of Pb, As, and Zn in contaminated soils and mine tailings, *G. Brown, Stanford*.
- Arsenic cycling in Bangladesh: solid phase species and mobilization mechanisms, A. Foster, US Geological Survey.
- Environmental chemistry of biogenic manganese-oxides, *J. Bargar, SSRL.*
- Selenium biotransformations in aquatic systems, S. Borglin, LBNL.
- Particulate matter and trace metals derived from fossil fuel, *G. Huffman, U. Kentucky.*
- Characterization of Cr, U, & Am in highly alkaline systems, L. Rao, LBNL.

Understanding Mercury in Fish using Synchrotron Radiation



Mercury pollution from paper mills, power plants, and garbage incinerators can wind up in rivers and oceans, where it accumulates in the tissue of fish.

Harris, Hugh H., Pickering, Ingrid J., George, Graham N. The Chemical Form of Mercury in Fish Science 2003 301: 1203http://www.sciencemag.org/cgi/content/full/301/5637/1203

Most researchers assumed the mercury that builds up in fish is <u>methylmercury</u> <u>chloride</u>, but no one knew for sure because the levels in fish were too low to study with traditional x-ray imaging techniques. Biophysicist Graham George of the University of Saskatchewan in Saskatoon, Canada, and his colleagues used a new high-intensity x-ray beam at the *Stanford Synchrotron Radiation Laboratory* in California to analyze the mercury in the muscle tissue of swordfish and orange roughy bought at a local seafood market. They found that the mercury in both fish is bound to a carbon atom and a sulfur atom and is most likely <u>methylmercury cysteine</u>, not methylmercury chloride.

This could be good news for consumers, because methylmercury cysteine may not be as adept at crossing cell membranes as the chloride form is, and so may be less toxic.

Growth of Molecular Environmental Science Activities at SSRL



*Scaled to 34.5 wk. year

Research Highlights from the Light Sources





Countering Bioterrorism. This past year, using the NSLS, SSRL and APS, researchers have determined the structures of two of the three components that constitute the anthrax toxin: proteins called Lethal Factor and Edema Factor. These structures give molecular insight into how anthrax causes infection and directly guide development of new drugs to defeat the anthrax threat.

Understanding the Molecular Machines of

Life. All cells contain remarkable cellular "machines," that decode genes to make proteins. Using data from each of the four synchrotrons, scientists have now determined the structures of two of these remarkable multi-component complexes (called polymerase and ribosome). Besides the remarkable discovery, these structural insights are leading to more effective strategies for designing new antibiotics.





Synchrotron Studies Used to Guide Development of New Process for Manufacture of Flat Panel Displays

Today's laptop computers utilize flat panel displays where the light transmission from the back to the front of the display is modulated by orientation changes in liquid crystal (LC) molecules. One of the key steps in the manufacture of the displays is the alignment of the liquid crystal molecules in the display. Today this is done by mechanical rubbing of two polymer surfaces and then sandwiching the LC between two such surfaces with orthogonal rubbing directions. Over the past years a great challenge of this \$10 billion/year industry has been to devise an alternative method of liquid crystal alignment. The rubbing process is plagued with contamination issues and the polymer film is deposited by a wet process that is incompatible with high-tech manufacturing techniques. The development of a new alignment technology, however, has been impeded by the fact that the origin of LC alignment has remained a mystery since its discovery in 1907.

- Polarization and surface sensitive spectroscopy measurements at SSRL by IBM scientists have been used to solve this puzzle.
- The <u>understanding of the molecular alignment</u> <u>mechanism</u> for rubbed polymer surfaces has directly led to the development of alternative alignment materials and processes which are discussed in three patents and described in <u>Science 292, 2299 (2001).</u>







Ultra-Sensitive Analysis of Metal Contamination on Silicon Wafer Surfaces

- Increasing the speed and complexity of integrated circuits requires advanced processes that put extreme constraints on the level of metal contaminants on silicon wafer surfaces.
- Synchrotron radiation from <u>SSRL</u> has been used to excite x-ray fluorescence from the metal contaminants with sensitivities as low as <u>one metal atom</u> <u>per 10⁷ silicon atoms</u>. This is 100x better than conventional techniques.
- This sensitivity meets the requirements of the Sematech Roadmap well into the 21st Century and the facility is being used regularly by the semiconductor industry.





Silicon Wafer



Materials Science



Osteoporosis Research

- Understanding Loss of Bone Mass



X-ray tomograph of trabecular bone in the human femoral neck taken with synchrotron radiation by LLNL scientists using synchrotron radiation at <u>SSRL</u> Osteoporosis is a major public health problem

- 1.3 million osteoporotic fractures each year
- 50% of women over 70 have had at least one fracture
- a disease which strikes without warning
- responsible for more deaths than breast cancer





before estrogen loss

after estrogen loss

Estrogen deficiency induces rapid bone loss and altered architecture. This can be visualized in living beings using non-invasive x-ray synchrotron tomography imaging. The image above is from a rat taken under sedation.

Vincent van Gogh, 1853 - 1890 Still life with meadow flowers and roses **Kröller-Müller Museum**



Under the flowers



BES Strategic Planning

10 workshops; 5 years; more than 1,500 participants from academia, industry, and DOE labs

Important Recurring Themes – Disruptive Technologies Require "Control" Control of materials properties and functionalities through electronic and atomic design

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- "Control" of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designer catalysts
- Designer interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation

Directing Matter and Energy: Five Challenges for Science and the Imagination

- Synthesize, atom by atom, new forms of matter with tailored properties Imagine: Create & manipulate natural & synthetic systems that will enable catalysts that are 100% specific & produce no unwanted byproducts, or materials that operate at the theoretical limits of strength & fracture resistance, or that respond to their environment & repair themselves like those in living systems
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
 Imagine: Master energy and information on the nanoscale, leading to the development of new metabolic and self replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision
 measurement tools as in molecular rulers, and defect-tolerant electronic circuits
- Control the quantum behavior of electrons in materials Imagine: Direct manipulation of the charge, spin and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun's energy into fuel through artificial photosynthesis.
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents

Imagine: Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO2 from atmospheric gases yet maintain high throughput.

Control matter very far away from equilibrium

Imagine: Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere. The Essential Role of Basic Science in Addressing the Energy Problem

- Today's energy technologies and infrastructure are rooted in 20th Century technologies and 19th Century discoveries—internal combustion engine, incandescent lighting.
- Current fossil energy sources, current energy production methods, and current technologies cannot meet the energy challenges we now face. These multifaceted challenges cannot be met by incremental improvements to existing technologies. Transformational changes and disruptive technologies – realized by pushing the frontiers of science – will be required.
- In the 20th century, scientists learned to observe and understand the interactions among atoms and molecules that determine material properties and processes. Now, scientists are poised to begin to direct and control the outcomes on an atom-by-atom and molecule-by-molecule basis. We don't yet know how to achieve these capabilities.
- 21st Century sciences and technologies will be rooted in the ability to direct and control matter down to the molecular, atomic, and quantum levels.

Central Dogma of Life







End of Presentation

Thank you



X-RAY PEAK BRIGHTNESS vs PULSE DURATION Past, Present, and Future

Peak Brightness [Phot./(s · mrad² · mm² · 0.1%bandw.)]


• Each FEL independently controlled in: wavelength, pulse duration, polarization

• Each FEL is configured with an optical manipulation technique: seeded, attosecond, ESASE Laser systems, timing & synchronization

Figure 2.3 Schematic of a light source facility based on a high-pulse-repetition-rate, seeded FEL.

Scientific Challenges for Future Light Sources, & Accelerator Research & Development Required to Meet Them; LBNL White Paper, July 14, 2006

Long Term Vision



FEL R&D for LCLS, LCLS-II, NGLS





INTERNATIONAL

Ambition, Challenges Shape S&T in Middle East, Northern Africa

Across the Middle East and North Africa, nations are embracing science as a way to drive economic development and improve the lives of their citizens. Some are investing heavily in universities and research centers, and several have space programs. Others are making strong commitments to science diplomacy.

But the region's researchers say they still face substantial challenges as they work to expand scientific capacity and pursue international partnerships. In a recent series of workshops cosponsored by AAAS and held in Jordan, Kuwait, Tunisia, and Dubai in the

The workshops, organized by the AAAS Center for Science, Technology and Security Policy with institutions in the four host countries, focused on best practices in international bioscience. Gwenaële Coat, asenior program associate at the AAAS center, said some participants attended all the meetings to encourage region-wide representation in these research fields and ensure "the impact of the meetings will last for many years."

At the first meeting in October 2010 in Jordan, the participants realized that the workshops also were an excellent place to discuss broader challenges for the region's ing [these] issues in their own communities," Almudhaf said, "and think that the decisionmakers will approach them first."

The workshops were especially valuable in highlighting some of these priorities, from clean water to infectious disease, which would benefit from stronger regional ties among researchers. "I think that there are a lot of learning opportunities between countries that have similar socioeconomic backgrounds and similar challenges," said Ayesha Abdullah, the managing director of Dubai Healthcare City. "But we don't yet have enough conferences and opportunities for networking."

Early career scientists who attended the last two workshops, held in Tunisia in November 2011 and in Dubai last March, spoke passionately about the need for more networking and mentorship.

"With young researchers, collaboration is easy to establish by Internet, but it's often limited to exchanging information," said Amel Benammar-Elgaaied, head of the genetics laboratory at the Faculty of Sciences of Tunis, Younger scientists, she said, need new ways to build relationships with established researchers in the region who are more likely to have financial and administrative support.

The researchers also have different needs depending on which country in the diverse area they come from, said Almudhaf. "The oil-rich countries in the Gulf might need more human resources" like mentors, she explained, "while in other parts of the region, funding is a critical factor."

These differences make it difficult to predict the Arab Spring's impact on young scientists, said Mona Mostafa Mohamed, the head of Cairo University's Cancer Biology Research Laboratory. In the North African countries at the epicenter of the uprising, she suggested, researchers who study abroad "for the time being might prefer to go and not to come back. They don't know how it's going to be yet."

Despite the uncertainties, the workshop participants pledged at the close of the Dubai workshop to write a collaborative article about their experiences and hold another regional conference in 2013. "I think with time, people will understand the importance of science and technology as a growth engine in developing countries," Abdulah said. "Science could be an answer to a lot of the challenges that the region faces." *Becky Ham*

Science Magazine June 29, 2012

Downloaded from www.sciencemag.org on July 30, 2012



Future vision. SESAME—Synchrotron-light for Experimental Science and Applications in the Middle East—represents the potential future of science and technology in the region. Now under construction in Jordan, the particle accelerator will foster ambitious, multidisciplinary research and build relationships across borders.

United Arab Emirates, the scientists said that young researchers in particular need better access to mentors, more opportunities to work with regional colleagues, and in some cases more funding and equipment. At the same time, they suggested, researchers must work closely with policy-makers to develop national scientific priorities.

"We can already see that governments and leaders in this part of the world are realizing that one of their best investments is to get younger people into science and technology," said Hayfaa Almudhaf, senior adviser to the director general of the Kuwait Institute for Scientific Research. scientists. Two months later, however, popular protests in Tunisia marked the start of the Arab Spring movement. Revolutionary demonstrations spread throughout the region, and by the time the second workshop was held in Kuwait in March 2011, the upheaval had added a new layer of uncertainty to the region's prospects in science and technology.

The researchers were hopeful that new governments would support a higher profile for science. But their discussions had a different focus: Apart from any political change, how should scientists become more active in aligning research goals with national priorities? "Scientists keep discuss-

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