X-ray Free Electron Laser

(Accelerator Based X-ray Laser)

Tsumoru Shintake

RIKEN/SPring-8

How does it work? How to use?

SCSS/XFEL Status April, 2010



Free Electron Laser Basic

About our SCSS & XFEL/SPring-8

Diffraction Imaging

SPring-8/XFEL and SCSS

Technology Transfer Thermionic Gun, injector, etc. SPring-8 Operating twelve years

January 2010

XFEL/SPring-8 Beam commissioning will start March 2011

SCSS Test Accelerator Since 2006, EVU user facility

Beam commissioning will start next year.

Expecting First FEL X-ray Lasing in 2011.

Experimental Hall

250 m Undulator Hall

400 m Linear Accelerator

Klystron Gallery

You are here

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Machine Assembly Hall klystron, modulators, accelerating structures,



Undulator = Periodic Magnetic Device



Understanding Radiation

- Free download "Radiation2D" from http://ShintakeLab.com
- Basic physics of radiation.
 - Radio-wave(dipole radiation)



- Thermal radiation.
- Synchrotron Radiation
- Undulator Radiation
- Free Electron Laser Basic







We need very high energy

Doppler shift

 $\lambda_{x} = ct - \lambda_{u}$ $= \left(c / \overline{u}_{z} - 1 \right) \lambda_{u}$ $= \left(1 / \overline{\beta}_{z} - 1 \right) \lambda_{u}$ $= \frac{\lambda_{u}}{2 \gamma^{2}} \left(1 + \frac{K^{2}}{2} \right)$

$$\gamma = E / m_0 c^2 = 8 \text{ GeV} / 0.51 \text{ MeV} = 15600$$

 $\beta = \sqrt{1 - 1/\gamma^2} \approx 1 - 1/2\gamma^2 = 1 - 2.05 \times 10^{-9}$
= 0.999999998

 $K = 0.1 \times \lambda_u(cm) \times B_x(kG)$ $= 0.1 \times 2cm \times 10kG)$ = 2

$$\lambda_x = \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{K^2}{2} \right)$$

$$=\frac{2cm}{2(15600)^2}(1+2^2/2)=0.4\dot{A}\times 3=1.2\dot{A}$$

Traveling time for one wavelength

 $1/\overline{\beta}_{z} - 1 \approx 1 - \overline{\beta}_{z}$

 $= (1 - \overline{\beta}_z) \times \frac{1 + \overline{\beta}_z}{1 + \overline{R}}$

 $=\frac{1}{2\gamma^2}\left(1+(\gamma\overline{\beta}_y)^2\right)$

 $=\frac{1}{2\gamma^2}\left(1+\frac{K^2}{2}\right)$

 $\approx \frac{1 - \overline{\beta}_z^2}{2} = \frac{1 - \beta^2 + \overline{\beta}_y^2}{2}$

 $t = \lambda_{\mu} / \overline{u}_{z}$

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FEL = Coherent Undulator Radiation



SCSS/XFEL Status
April, 2010

Physical Origin of Micro-bunching (FEL Action)

Undulator field produces curved trajectory. From this slope, the tangential component of EM wave creates longitudinal field.





Distance Along Undulator

T. Shintake 2007.01

Basic Machine Layout of XFEL/SPring-8



Expected Performance of XFEL/SPring-8



SCSS : SPring-8 Compact SASE Source



SCSS Test Accelerator Performance

- 2006 First lasing at 49 nm
- 2007 Full saturation at 60 nm
- 2008 User operation stat

500 kV Pulse electron gun CeB6 Thermionic cathode Beam current 1 Amp.

In-vacuum undulator C-band accelerator S-band buncher 476 MHz booster 238 MHz buncher E-beam Charge: 0.3 nC Emittance: 0.7 π .mm.mrad (measured at undulator) Four C-band accelerators 1.8 m x 4 Emax = 37 MV/mEnergy = 250 MeV **In-Vacuum Undulators**

Period = 15 mm, K=1.3 Two 4.5 m long. Single-crystal CeB₆ Cathode for the SCSS Low-emittance Injector

No HV breakdown for 4 years daily operation



500 kV Electron Gun









Diameter : ϕ 3 mm Temperature : ~1500 deg.C Beam Voltage : 500 kV Peak Current : 1 A Pulse Width : ~2 µs

Heating Cathode



It was found the cathode surface became concave of 0.2 mm deep from the initial flat surface. It corresponds to evaporation speed of 10 nm/hour (10 nm/h x 20,000 h = 200 micron-meter) Concave geometry made beam slightly focusing, but did not break emittance. Electron microscope study showed (1) Surface is fairly smooth, (2) covered by carbon contamination (lowered electron emission).

Measured Emittance at the Gun

Beam Profile

ф 5.6 mm (FWHM)

20 mm



Phase Space Profile

Beam energy	500 keV
Peak current	1 A
Pulse width (FWHM)	3 µs
Repetition rate	10 Hz
Normalized emittance (rms, 100% electrons)	1.1π mm mrad
Normalized emittance (rms, 90% electrons)	0.6π mm mrad
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20 mm

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CeB₆ Thermionic Gun provides stable beam.

Beam Profile CCD Image Scale 10 mm



250 MeV Compressor

Undulator Input

Undulator Output

July 2007, Stockholm

First Lasing at SCSS Prototype Accelerator.



First Lasing at SCSS Prototype Accelerator.



- The first lasing: 49 nm
- E-beam energy : 250 MeV
- Bunch charge: 0.25 nC
- Bunch length: (< 1 pse)
- Peak Current (> 300 A)

 At moment spectrum width 0.5 nm is dominated by e-beam energy fluctuation ~ 0.2%.



MATERIALS SCIENCE

Japanese Latecomer Joins Race To Build a Hard X-ray Laser

X-ray free-electron lasers are the next big thing in high-energy probes of matter. With U.S. and European machines in the works, Japan wants into the club

SAYO, HYOGO PREFECTURE, JAPAN—It's the scientific version of keeping up with the Joneses. Once researchers in one region plan a big, new experimental device, researchers everywhere want their own. The latest example: x-ray free-electron lasers (XFELs), which promise beams that are vastly brighter and with higher energy and shorter pulses than today's workhorse synchrotron x-rays.

These "hard" x-ray wavelengths—down to 0.1 nanometer—promise to reveal the struc-

broad interest for science, it is no surprise that [researchers] in three regions of the world want to have a facility of their own," says Reinhard Brinkmann, who leads the European effort based at the German Electron Synchrotron (DESY) research center in Hamburg. "Freeelectron lasers are amazing things which herald a new era in photon science," says Janos Hajdu, a synchrotron radiation specialist at Uppsala University in Sweden.

XFELs rely on new approaches to gener-

SCIENCE VOL 314 3 NOVEMBER 2006

or oscillating in lockstep—a quality missing from synchrotron light.

Although all three planned systems share the same basic setup, subtle differences give each of them strengths and weaknesses. "The final targets of the XFEL projects are the same, but the means are different," says Tsumoru Shintake, who heads accelerator development for Japan's XFEL.

The first project to come online will be Stanford's LCLS. Much of the key research underpinning XFELs was done at SLAC beginning in the early 1990s. And SLAC got a head start by using a 1-kilometer stretch of its now-idled linear accelerator, or linac. The SLAC group estimates that reusing its linac has saved more than \$300 million, giving a total construction cost of \$379 million. LCLS will have one undulator providing hard and soft x-rays to up to six experimental stations. Galayda says the group expects to generate its first x-rays by July 2008 and to start experiments by March 2009.

Japan's entry is the SPring-8 Compact SASE Source (SCSS), just now getting under construction here. Latecomers to the field, the team is using some homegrown technology to cut cost and size. "We're taking the first step toward making XFELs smaller and cheaper so more [institutions] can consider developing their own," boasts SCSS project leader Tetsuya Ishikawa. Whereas the other two machines will generate electrons by firing a laser at a metal target, the SCSS heats a cathode to produce electrons. Eliminating the laser simplifies the system but requires careful compression of the cloud of electrons before they go into the linac.

The wavelength of the output x-rays is a tradeoff between the energy of the electrons

It's laser light at EUV



60 nm, courtecy of Nishino.

SCSS	/XFEL	Status
April,	2010	

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Status of XFEL/SPring-8 Construction

	FY'06	FY'07	FY'08	FY'09	FY'10) FY'11
Building	-	Accelerator Undulator	Tunnel Hall	Experimer Hall	ntal	
Accelerating structures and waveguide systems	E		Production	Installat	tion	
Klystrons and modulators	Klystro Mo	n dulator <	Producti	on		
Control cabinets and			Produ	Install Iction		
low level rf systems				Instal	lation	eam
Undulators				Productic Inst ◀	allation	t X-ray B
Beam Commissioning		H	igh power Beam	rf proces Commis	sing - sioning	Firs

50 m Experimental Hall

200 m Undulator Hall

400 m Accelerator Tunnel

Klystron Gallery

Machine Assembly Hall

Experimental Hall



SCSS/XFEL Status April, 2010

Beam Lines

Beamline

5 beamlines (final) Start from BL3 (XFEL) & BL1 (SX)

4 Experimental Hutches EH1: R&D EH2: Pump & Probe EH3: Imaging EH4: Open hutch Laser booth

Laser booth (CPA, OPA)

SX

BL3

HX

SX HX HX

7 m

相互利用基盤 XFEL+SR

Accelerator installation







SCSS/XFEL Status April, 2010

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April, 2010

C-band Accelerator for Multi-bunch Option



T. Shintake, "Choke Mode Cavity", Jpn. J. Appl. Phys. Vol. 31 pp. L1567-L1570, November 1

Higher Order Mode Damping for Multi-bunch operation. Maximum 50 bunches x 1 nC, at 4.2 nsec spacing

X-ray 4.2 nsec x 50 bunches will be key for Single bio-molecule imaging to improve Luminosity.



13,000 cells are under mass production.



Sadao Miura, MITSUBISHI Heavy Ind, April 2008

HITACHI Cable Co. completed mass production of C-band cell. June 2009

We made 13,000 pieces of C-band accelerator cell.

Mass Production of C-band Accelerator at MITSUBISHI Heavy Ind. 2007 ~ 2009



MITSUBISHI-Team completed 100 tubes (out of 128) C-band Accelerator. Photo March 2009



Testing Modulator & Klystron



SCSS/XFEL Status April, 2010 Tsumoru Shintake shintake@spring8.or.jp
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May 2010

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SCSS/XFEL Status April, 2010

Beam Monitor Devices

By Y. Otake team.



All undulators (18) have been installed in Augost

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Undulator is ready for mass production.

T. Shintake@ SCSS & XFEL/SPring-8 2009

Undulator for XFEL/SPring-8

Outlook of 5 m long in-vacuum undulator for X-ray FEL.

NeFeB magnet array, undulator period is 18 mm.

Undulator for XFEL/SPring-8

Undulator Type		In-Vacuum Planer Undulator
Active Length		5 m
Undulator Period		18 mm
Magnetic Circuit		Hybrid (NdFeB+Permendur)
Peak Field	Maximum	1.31 T
	Nominal	1.13 T
К	Maximum	2.2
	Nominal	1.9
Gap	Minimum	3.5 mm
	Nominal	4.5 mm
Maximum Attractive Force		~ 6 ton

Why we are constructing XFELs?

- Realize dream of laser at X-ray wavelength.
- Very high peak power 2 GW, high photon flux.
- Very short pulse length. < 100 fsec</p>
- Widely tunable wavelength.

Peak Brilliance Evolution



Peak brilliance will be enhanced by factor of 10¹⁰ from 3rd generation SR to XFEL.

 $10^{10} = 10^1 \times 10^1 \times 10^1 \times 10^7$

peak current by factor 10
x lowered emittance by 10
x energy spread lowered by 10
x interference effect 10⁷ by microbunching formation.

XFEL Radiation Characteristics

High Peak Power ~ GW

→ high field non linear physics

→ high flux photons for single shot diffraction imaging

single molecular structural analysis

 Short Pulse 10 ~ 100 fsec
 Time resolving experiment (Pump probe) Chemical reaction

Coherent → Holography, Coherent Imaging

Why 1 Angstrom?



Photo-ionization becomes lower as X-ray energy.

- Around 1 A, 8 keV, photoionization becomes low enough to see coherent scattering.
- Spatial resolution becomes a few Angstrom, which resolves macromolecular crystal in biology.

→ Imaging, crystallography

water window (2.3-4.4nm light) is also another candidate.
 (a few micron-meter thick water)



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Science with X-ray Free Electron Laser









X-ray Diffraction Pattern

Coherent diffraction imaging







Optical Microscope



Lensless Diffraction Microscope



Glass Bead (Single Lens) does Microsope



April, 2010





Iterative Phase Retrieval



Fienup, J.R. 1978. Reconstruction of an object from the modulus of its Fourier transform. Optics Letters, 3: 27-29





Fig. 3. (A) Diffraction pattern recorded with a single FEL pulse from a test object placed in the 20- μ m focus of the beam (β). (B) The diffraction pattern recorded with a second FEL pulse selected with a fast shutter, showing diffraction from the hole in the sample created by the first pulse. (C) Scanning electron microscope image of the test object, which was fabricated by ion-beam milling a 20-nm-thick silicon nitride membrane. The scale bar denotes 1 μ m. (D) The image reconstructed from the single-shot diffraction pattern shown in (A).

Chapman, H.N., A. Barty and M. Bogan et al. 2006. Femtosecond diffractive imaging with a soft-X-ray free-electron laser, Nature Physics 2: 839-843

Possibility of single biomolecule imaging with coherent amplification of weak scattering x-ray photons

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The number of photons produced by coherent x-ray scattering from a single biomolecule is very small because of its extremely small elastic-scattering cross section and low damage threshold. Even with a high x-ray flux of 3×10^{12} photons per 100-nm-diameter spot and an ultrashort pulse of 10 fs driven by a future x-ray free electron laser (x-ray FEL), it has been predicted that only a few 100 photons will be produced from the scattering of a single lysozyme molecule. In observations of scattered x rays on a detector, the transfer of energy from wave to matter is accompanied by the quantization of the photon energy. Unfortunately, x rays have a high photon energy of 12 keV at wavelengths of 1 Å, which is required for atomic resolution imaging. Therefore, the number of photoionization events is small, which limits the resolution of imaging of a single biomolecule. In this paper, I propose a method: instead of directly observing the photons scattered from the sample, we amplify the scattered waves by superimposing an intense coherent reference pump wave on it and record the resulting interference pattern on a planar x-ray detector. Using a nanosized gold particle as a reference pump wave source, we can collect $10^4 - 10^5$ photons in single shot imaging where the signal from a single biomolecule is amplified and recorded as two-dimensional diffraction intensity data. An iterative phase retrieval technique can be used to recover the phase information and reconstruct the image of the single biomolecule and the gold particle at the same time. In order to precisely reconstruct a faint image of the single biomolecule in Angstrom resolution, whose intensity is much lower than that of the bright gold particle, I propose a technique that combines iterative phase retrieval on the reference pump wave and the digital Fourier transform holography on the sample. By using a large number of holography data, the three-dimensional electron density map can be assembled.

DOI: 10.1103/PhysRevE.78.041906

PACS number(s): 87.85.Ng, 42.30.Rx, 07.85.Tt, 42.40.Ht

T.Shintake 2009.Feb

Physical Origin of Difficulty

- In observations of scattered X-rays on a detector, the transfer of energy from wave to matter is accompanied by the quantization of the photon energy. Unfortunately, X-rays have a considerably high photon energy of 12 keV at wavelengths of 1 Å, which is required for atomic resolution imaging.
- Therefore, the number of photoionization events is considerably less, which limits the resolution of the imaging of a single biomolecule.









t = -50 fs

Figure 2 Explosion of T4 lysozyme (white, H; grey, C; blue, N; red, O; yellow, S) induced by radiation damage. The integrated X-ray intensity was 3×10¹² (12 keV) photons per 100nm diameter spot $(3.8 \times 10^6 \text{ photons per Å}^2)$ in all cases. **a**, A protein exposed to an X-ray pulse with an FWHM of 2 fs, and disintegration followed in time. Atomic positions in the first two structures (before and after the pulse) are practically identical at this pulse length

because of an inertial delay in the explosion. $R_{\text{nucl}} = 3\%$, $R_{\text{elec}} = 11\%$ **b**, Lysozyme exposed to the same number of photons as in a, but the FWHM of the pulse was 10 fs. Images show the structure at the beginning, in the middle and near the end of the X-ray pulse. $R_{nucl} =$ 7%, $R_{\text{elec}} = 12\%$ **c**, Behaviour of the protein during an X-ray pulse with an FWHM of 50 fs. $R_{\rm nucl} = 26\%, R_{\rm elec} = 30\%.$







Figure 3 Elastic scattering from a variety of samples. **a**–**c**, Simulated diffraction images on a 128×128 pixel planar detector ($100 \text{ mm} \times 100 \text{ mm}$) normal to and centred at the beam, and placed 100 mm from the sample. The background was not modelled, and 100% detective quantum efficiency was assumed. The integrated X-ray intensity was 3×10^{12} (12 keV) photons per 100-nm diameter spot (3.8×10^6 photons per Å²); the pulse length was 10 fs. The resolution is 2.2 Å at the rim in **a**–**c**. cpp, counts per pixel. **a**, Scattering from a single tomato bushy stunt virus capsid. **b**, Scattering from a $5 \times 5 \times 5$ cluster of lysozyme molecules with an average r.m.s. conformational deviation

of 0.2 Å to model an imperfect lattice. **c**, Scattering from a single molecule of lysozyme. **d**, A planar section through the molecular transform (that is, a simulated continuous scattering image) of a single T4 lysozyme molecule under ideal conditions without sample movement or damage. Resolution at the rim of **d** corresponds to 2.0 Å. Structure factor amplitudes are coloured logarithmically (magenta, high; green, low). The section is perpendicular to the *z* axis, and crosses through the origin at the centre of the image, revealing centric symmetry.

Single Biomolecule Imaging with XFEL

(Heterodyne Detection + Holographic Recording)

"Weak diffraction from biomolcule is amplified by $10 \sim 50$ times (Heterodyne) on the coherent reference wave from nano-particle, providing 100~1000 times more photons" T. Shintake, PR-E 78, 041906 (2008) X-ray FEL Beam **Single Biomolecule** Heterodyne Amplification **Nano Particle of Heavy Atoms** Holographic as Coherent Reference Wave Source Recording

X-ray Heterodyne Detection T. Shintake 2003

• X-ray heterodyne detection using reference X-ray P1 on the small signal P2

$$P_{\pm} = \left(\sqrt{P_1} \pm \sqrt{P_2}\right)^2 = P_1 \pm 2\sqrt{P_1P_2} + P_2$$

$$= P_1 \left(1 \pm 2\sqrt{P_1/P_2} + P_1/P_2\right)$$

$$\approx P_1 \left(1 \pm 2\sqrt{P_1/P_2}\right)$$
Incident Wave Object Diffracted Wave Reference Wave P_1 Detector

• Even if P₂ is 10⁻⁶ times smaller, the signal is amplified to 10⁻³ level. This is +30 dB amplification.

Does noise increase or decrease?

- S/N due to the electrical noise in detector instrument can be easily improved as the signal growing.
- Question is the statistical noise associated with quantization of energy in photo-ionization process in CCD or film detector.
- Since amplitude of the interference pattern increase as $\infty \sqrt{I}$, and statistical noise also increases as $\infty \sqrt{I}$, thus S/N becomes constant, and looks like not been improved.

$$S / N |_{\text{holography}} = S / N |_{\text{direct}}$$

ND Filter X1/200









FIG. 4. (Color online) Conceptual diagram of a single lysozyme molecule linked to a gold particle (diameter of atoms is not drawn to scale). The gold particle produces 200 times more coherent x-ray scattering than the single lysozyme molecule. The bar at the bottom of the figure represents a four-slit thought experiment.

Fourier transform holography uses spherical waves as reference waves to record the phase of an object wave. The intensity of the reference wave is chosen such that it is comparable to that of the object wave to obtain the best contrast. To obtain better image quality, the size of the reference wave source should be considerably smaller than the object. The image-recovery process in Fourier transform holography is where $\Delta \phi_{ij} = \phi_j - \phi_i$ is the phase difference given by

$$\Delta \phi_{ij} = \phi_j - \phi_i = \frac{2\pi d_{ij}}{\lambda} \sin(2\theta).$$
(8)

Here, I_i represents the flux from the *i*th slit, 2θ is the scattering angle (as defined in crystallography), and d_{ij} is the distance between the *i* and *j*th slits. The slit locations and flux ratio suitable for our example case shown in Fig. 4 are as follows: $d_{12}=1.5$ nm, $d_{23}=8.5$ nm, $d_{34}=2$ nm, $I_1=200$, $I_2=10$, $I_3=1$, $I_4=0.1$, and $\lambda=1$ Å. Figure 5(a) shows the flux density distribution estimated using Eq. (7). The distribution is considerably complicated because the fringes are formed by the interference of four waves.

In Fig. 5(c), the curve at the bottom indicates the scattered wave from the biomolecule when it is directly observed without using the reference pump wave. It is a very weak signal with a relative intensity of approximately 1. In practice, the signal is quantized by the photon energy, leading to a loss of detailed information. The dashed curve (magnified 10 times) also shows an interference pattern, which represents the internal structure of the biomolecule; our aim is to study this pattern. By superposition of the reference pump wave, the signal wave is amplified, and the resulting interference pattern is recorded. In order to demonstrate the amplification effect clearly, the reference pump wave is assumed to be perfect with $\psi_2=0$. In Fig. 5(c), the curve at the top shows the amplified signal, which is recorded by the
File FFT Action Image Monitor PhaseMonitor PhaseSolver PhaseDet CrossCheck



Shintake, Summer 2008

Who is Shintake?



@ SCSS tunnel Test Accelerator for XFEL

 2006~ Now constructing 8 GeV XFEL/SPring-8 for 0..1 nmm wave

Shintake, Summer 2008













Design accelerator as creating images like art



Shintake, Summer 2008

Klystron Modulator for C-band, S-band 50 MW Klystrons



Compact Modulator for 50 MW Klystrons

- Output Power 50 MW RF x 60 pps
- 50 kV PFN, 1:16 Trans, 350 kV klystron.
- Compact 1 m x 1 m x 1.5 m,
- Very low noise (<10 Vpp on 200 V heater line)
- Water cooled. Max surface temp 45 deg.









Summary

- So many different efforts are coherently contributing to the project. They are almost on the time schedule.
- Building construction has been completed.
- Accelerator component installation has been started.
 ~ 1 year installation.
- October 2010, We start high power operation of accelerator.
- Spring 2011, we start beam commissioning.