**Cheiron School 2009** 

# X-ray Free Electron Laser

## **Tsumoru Shintake**

XFEL/SPring-8 Accelerator R&D Technical Director Main Accelerator Construction Leader SPring-8 Center, RIKEN

May 09 2009

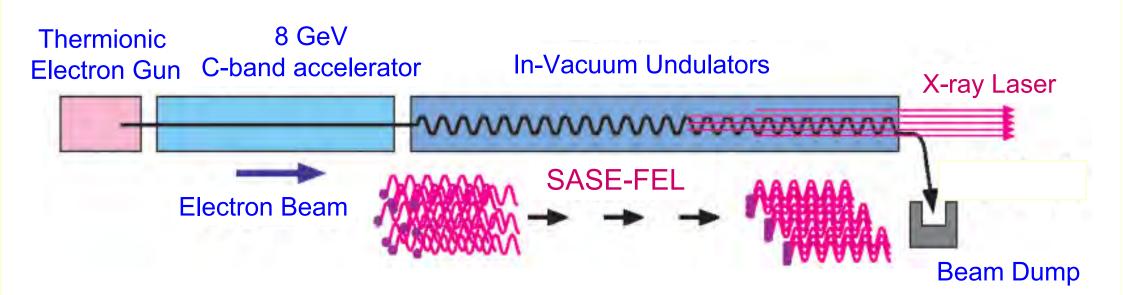
#### SPring-8 Operating ten years

XFEL/SPring-8 Building construction completed March 2009

> SCSS Test Accelerator Since 2006, EVU user facility

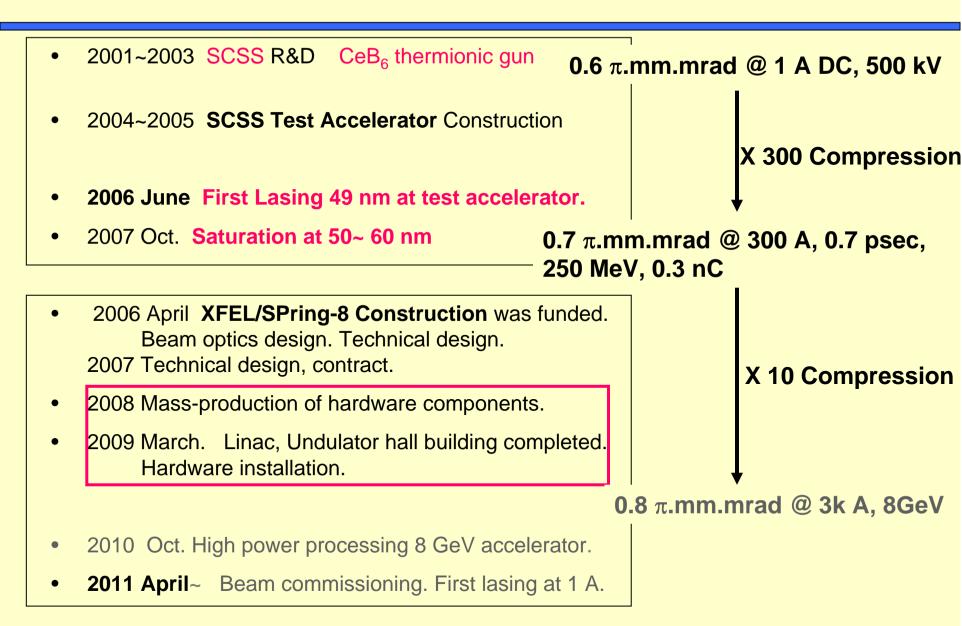
# **Concept of XFEL/SPring-8**

X-ray FEL



1) Electron gunLow emittance ( $\epsilon_N \sim 0.7\pi$  mm\*mrad)<br/>Higher electron density at the undulator.2) C-band acceleratorHigh gradient (Ea ~ 35 MV/m)<br/>Compact accelerator.3) In-vacuum undulatorShort period ( $\lambda_u \sim 18$  mm)<br/>Shorter wavelength<br/>with lower electron energy.

# SCSS to XFEL/SPring-8 Timeline



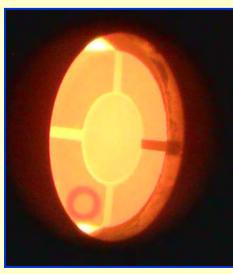
Single-crystal CeB<sub>6</sub> Cathode for the SCSS Low-emittance Injector

No HV breakdown for 4 years daily operation

500 kV Electron Gun

After 20,000 hours operation 1 crystal changed.







Diameter :  $\phi$ 3 mm Temperature : ~1500 deg.C Beam Voltage : 500 kV Peak Current : 1 A Pulse Width : ~2 µs **Heating Cathode** 

# Use Small Size Cathode ... First Strategy for smaller thermal emittance

Thermionic cathode

•



**3***mm* diameter cathode (CeB6) is used in a low emittance injector. (SCSS SPring-8/RIKEN)

Operating Temperature 1450°C  $w_e = \frac{3}{2}k_B T = 223 \text{ meV}$ 

Thermal Emittance

$$\varepsilon_{xN} = \frac{\gamma r_c}{2} \sqrt{\frac{k_B T}{m_0 c^2}} = 0.4 \ \pi \text{ mm-mrad}$$

 $0.28 \pi$  mm-mrad/mm

*RF* photo-cathode injector. Today's RF photo injectors use ~ 1 mm spot radius.  $\varepsilon_{xN} = \frac{\gamma r_c}{2} \sqrt{\frac{k_B T_e}{m_e c^2}} = 0.35 \pi \text{ mm-mrad}$ Same order!

 $T_e$  is "measured" effective electron temperature of copper *cathode using 266 nm laser (ref. 2).*  $k T_e = 0.27 \ eV \ (2360^{\circ}C)$ .



#### 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

# SCSS Test Accelerator Performance

238 MHz

buncher

- 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.

E-beam Charge: 0.3 nC Emittance: 0.7  $\pi$ .mm.mrad (measured at undulator)

In-vacuum

undulator

C-band

S-band

buncher

476 MHz

booster

accelerator

Four C-band accelerators 1.8 m x 4 Emax = 37 MV/m Energy = 250 MeV

In-Vacuum Undulators Period = 15 mm, K=1.3 Two 4.5 m long.

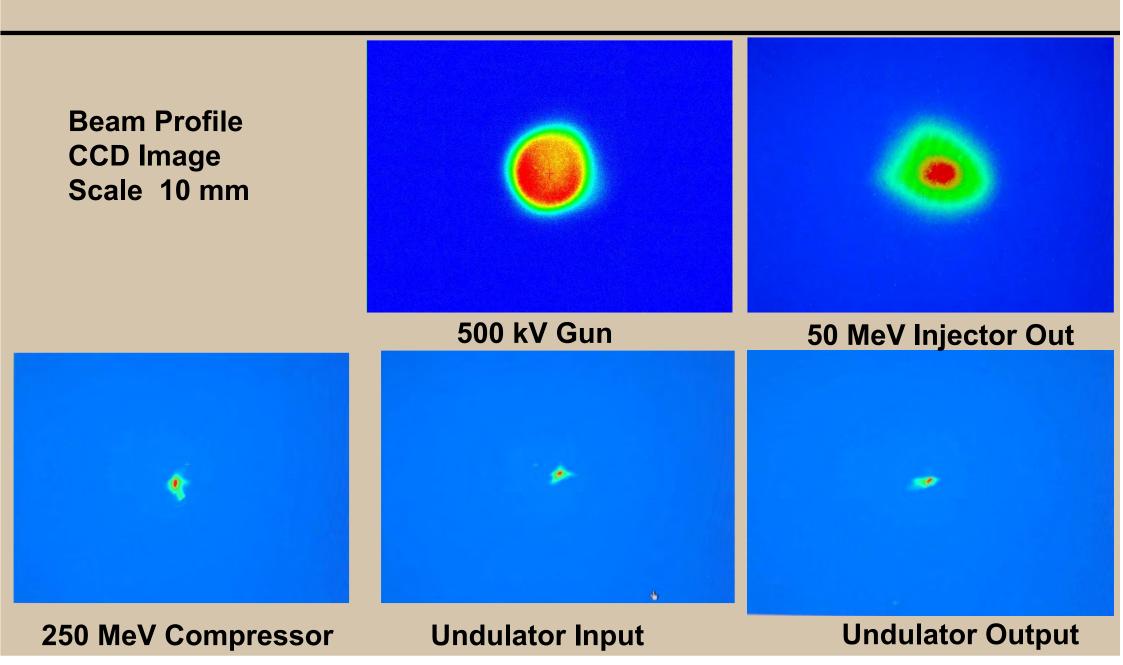
#### July 2007, Stockholm

# First Lasing at SCSS Prototype Accelerator.



T. Shintake, FEL06

# **CeB**<sub>6</sub> Thermionic Gun provides stable beam.

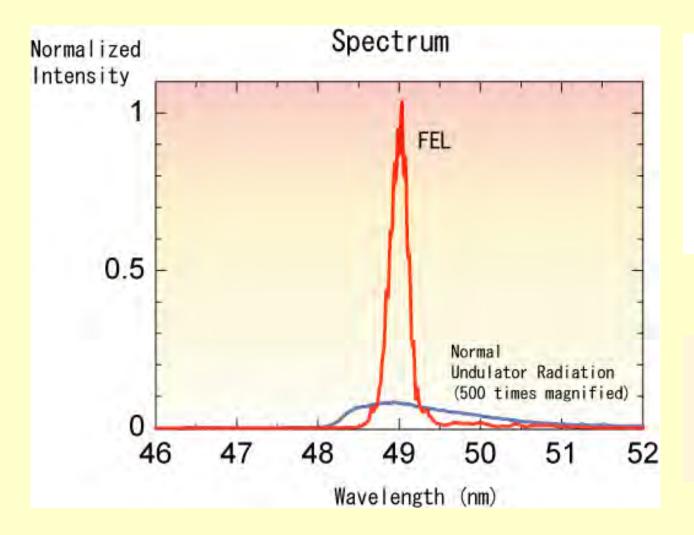


#### July 2007, Stockholm

# 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)

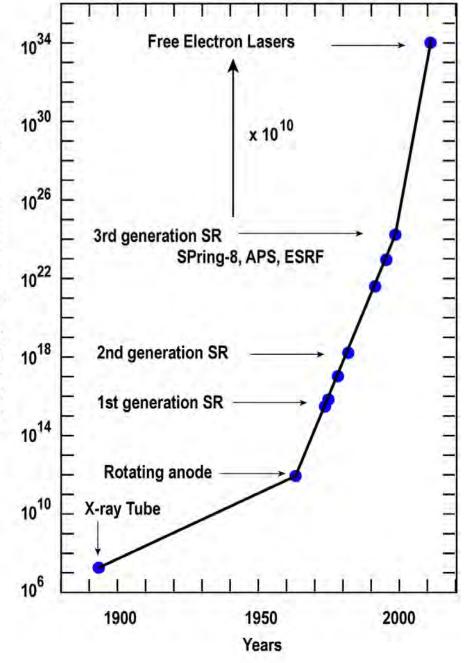
 At moment spectrum width 0.5 nm is dominated by e-beam energy fluctuation ~ 0.2%.

T. Shintake@ SCSS & XFEL/SPring-8 2008

# SCSS Test Accelerator User Run Has been Started in 2008

- 50~60 nm, 30 µJ/pulse
- Multi-photon absorption
- Coherent diffraction imaging
- etc.

# **Peak Brilliance Evolution**

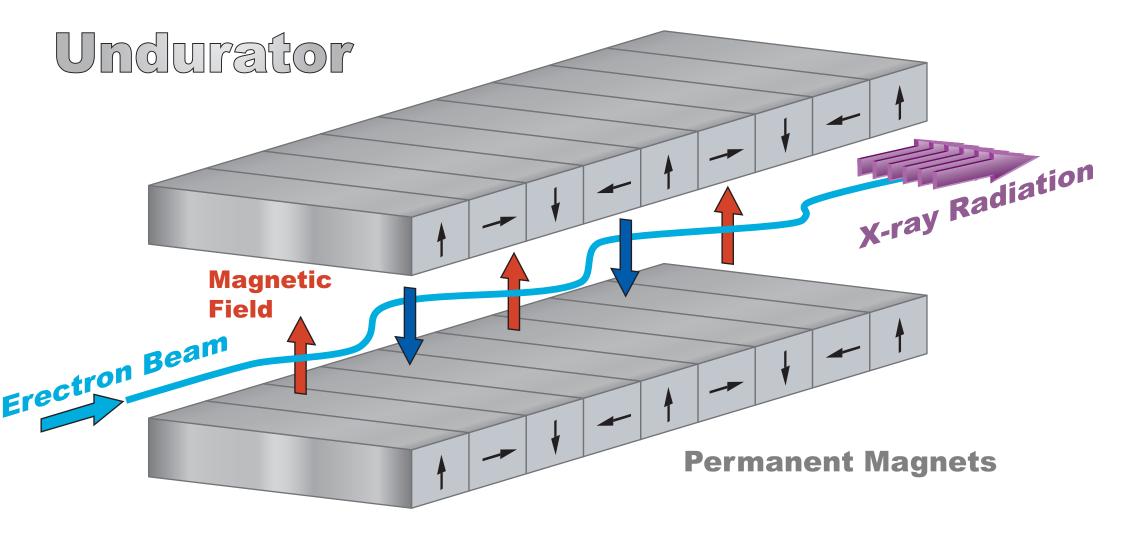


 Peak brilliance will be enhanced by factor of 10<sup>10</sup> from 3<sup>rd</sup> generation SR to XFEL.

PAC2007

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

peak current by factor 10
x lowered emittance by 10
x energy spread lowered by 10
x interference effect 10<sup>7</sup> by
micro-bunching formation.

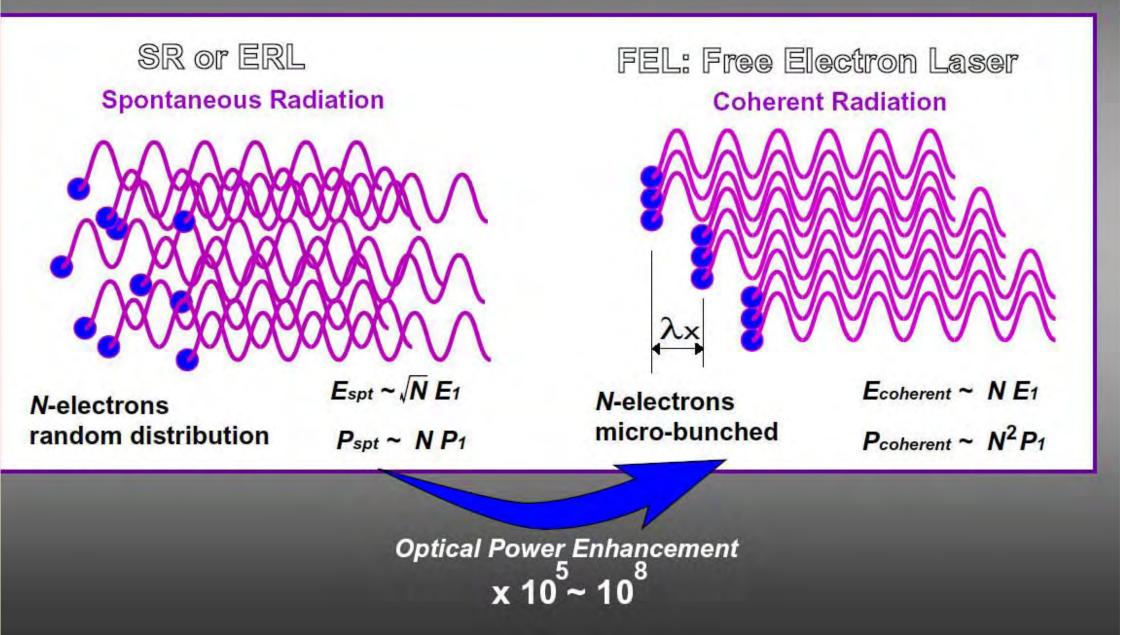


# Freeware Radiation2D is available at http://ShintakeLab.com

Terre & Shintake Lab

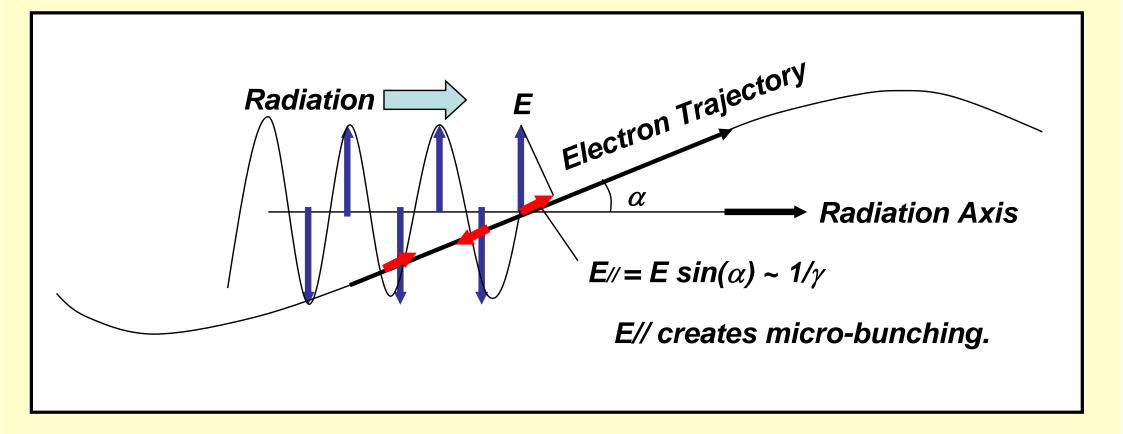


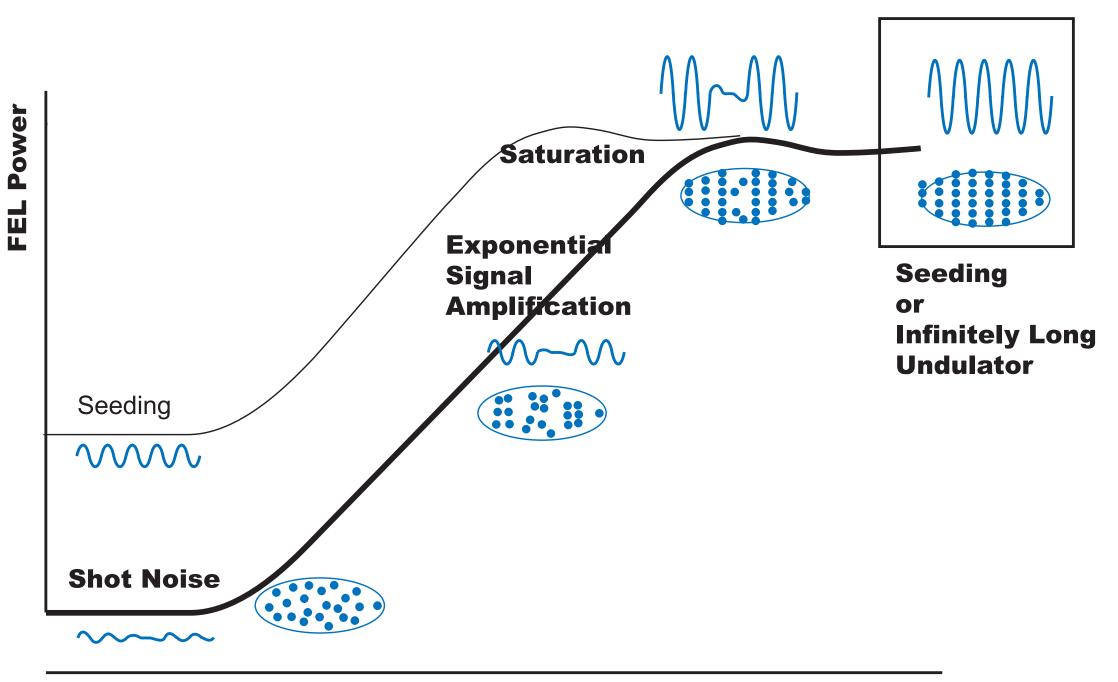
# From SR to FEL



# **Physical Origin of Micro-bunching (FEL Action)**

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

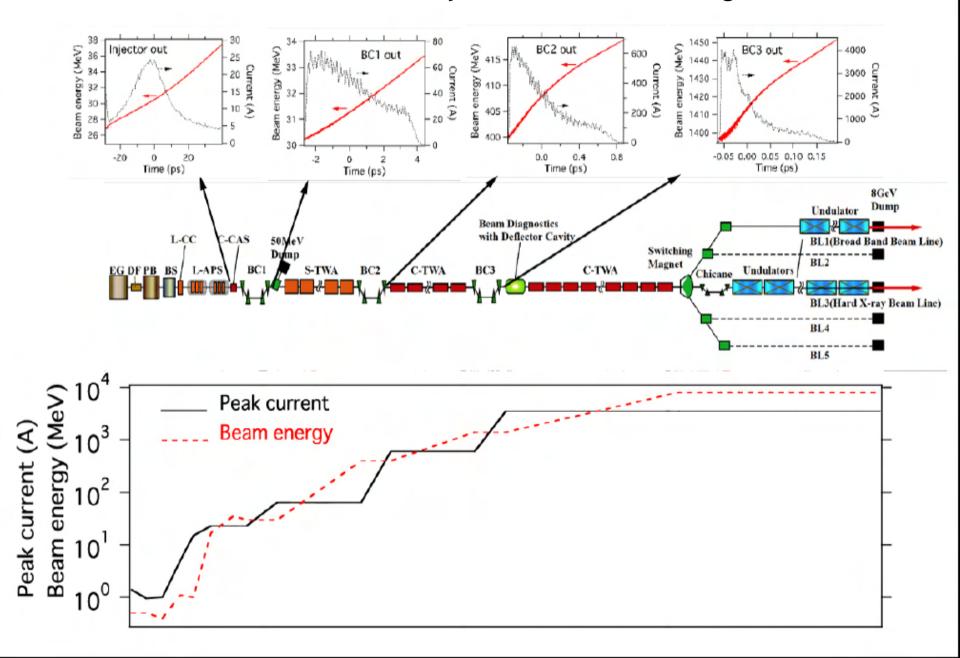




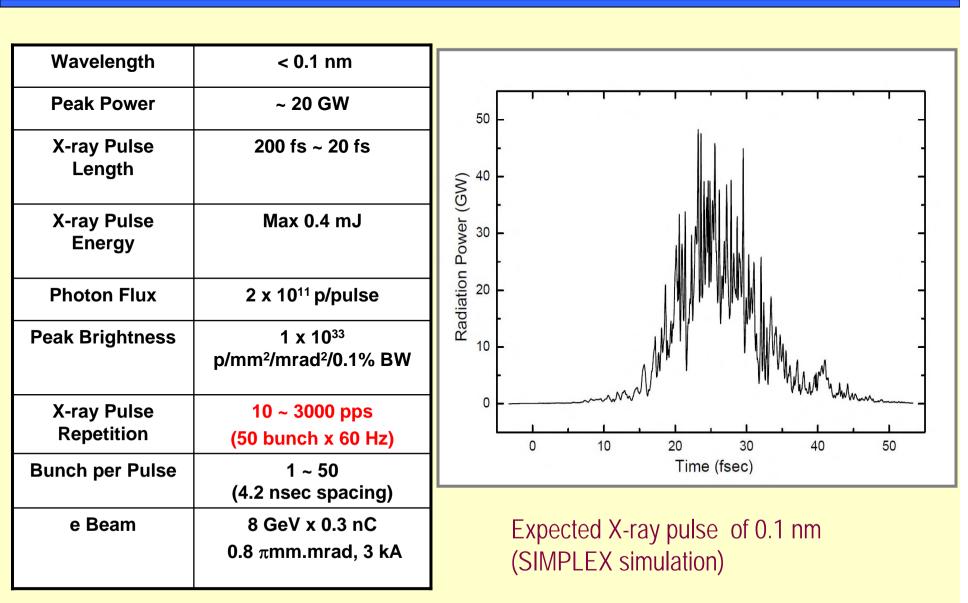
#### **Distance Along Undulator**

T. Shintake 2007.01

## **Basic Machine Layout of XFEL/SPring-8**



## **Expected Performance of XFEL/SPring-8**



XFEL/SPring-8 Building construction completed March 2009

Experimental Hall (under construction)

**Undulator Hall** 

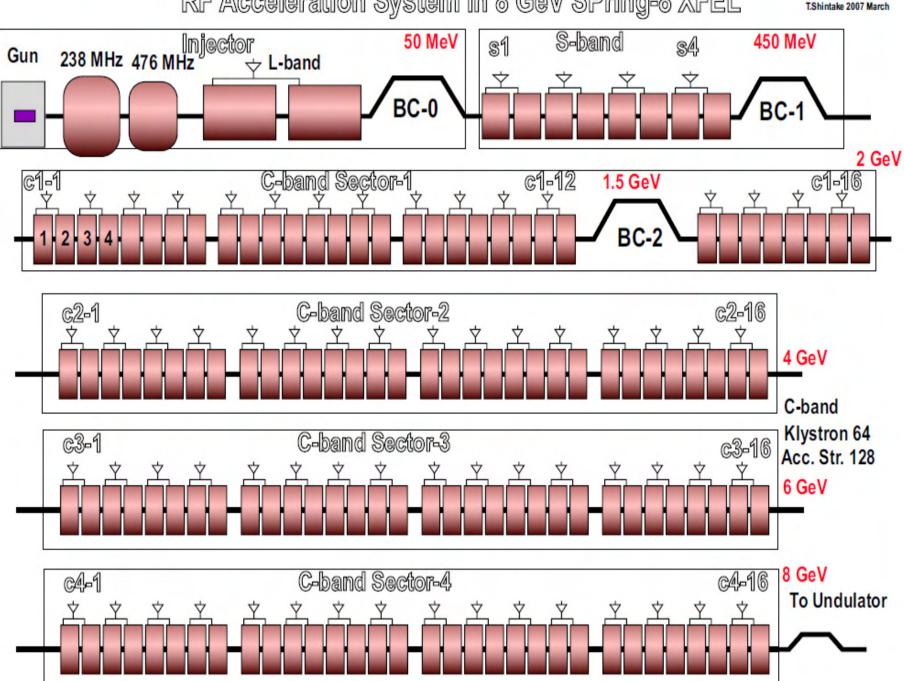
10000

#### 400 m Accelerator Tunnel

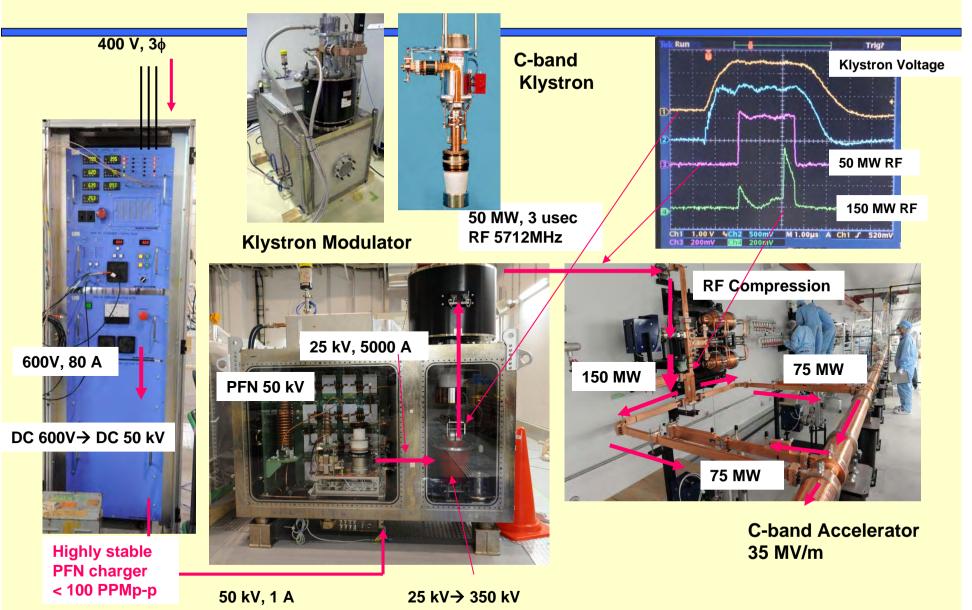
**Klystron Gallery** 

Machine Assembly Hall

RF Acceleration System in 8 GeV SPring-8 XFEL

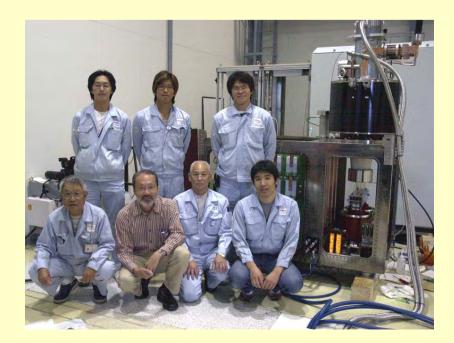


# **C-band System Configuration**



## **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)</li>
- Water cooled. Max surface temp 45 deg.





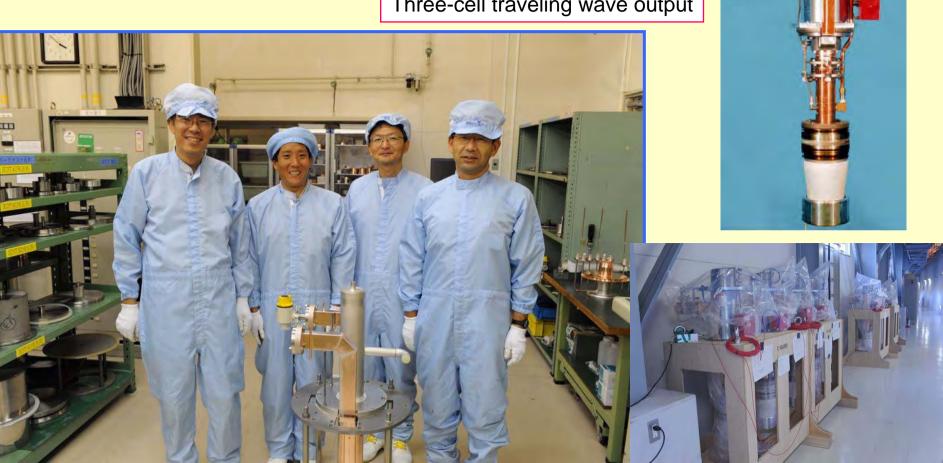
# Modulators are Arriving to XFEL/SPring-8

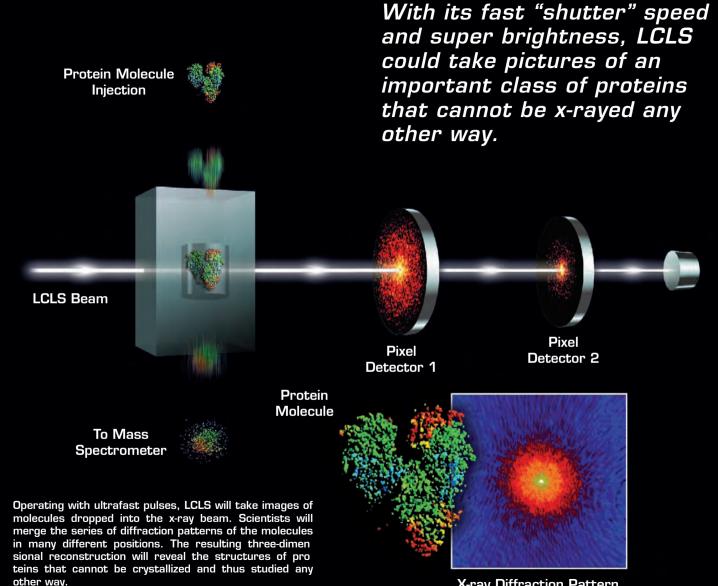


## Mass Production of Klystrons at TOSHIBA

- 64 C-band klystron
- 4 S-band klystron
- 1 L-band klystron

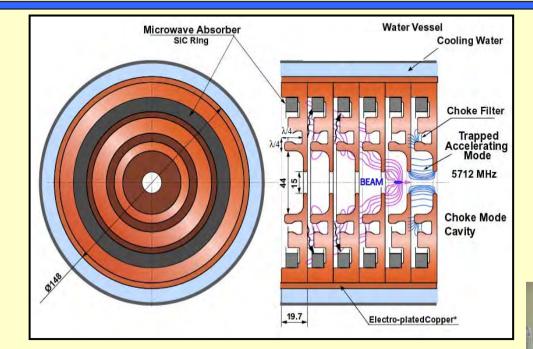
C-band Klystron 5712 MHz, 50 MW 4 µsec, 60 pps 45 % efficiency Three-cell traveling wave output





X-ray Diffraction Pattern

## C-band Accelerator for Multi-bunch Option



T. Shintake, "Choke Mode Cavity", Jpn. J. Appl. Phys. Vol. 31 pp. L1567-L1570, November 19

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 20

# 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

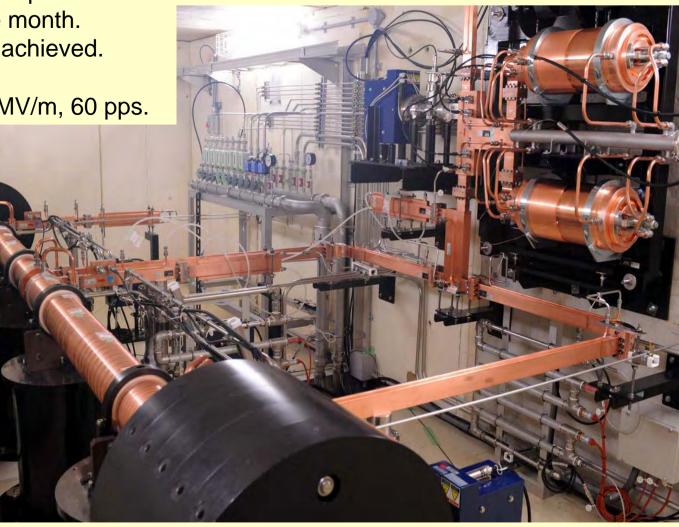


## MITSUBISHI-Team completed 100 tubes (out of 128) C-band Accelerator. Photo March 2009



## **Routinely Operation: C-band High Gradient Test**

- Sample test from mass production.
- C-band 1 unit for one month.
- **35 MV/m** is routinely achieved. (Very low trip rate.)
- Processing up to 40 MV/m, 60 pps.
- T. Sakurai, PAC2009



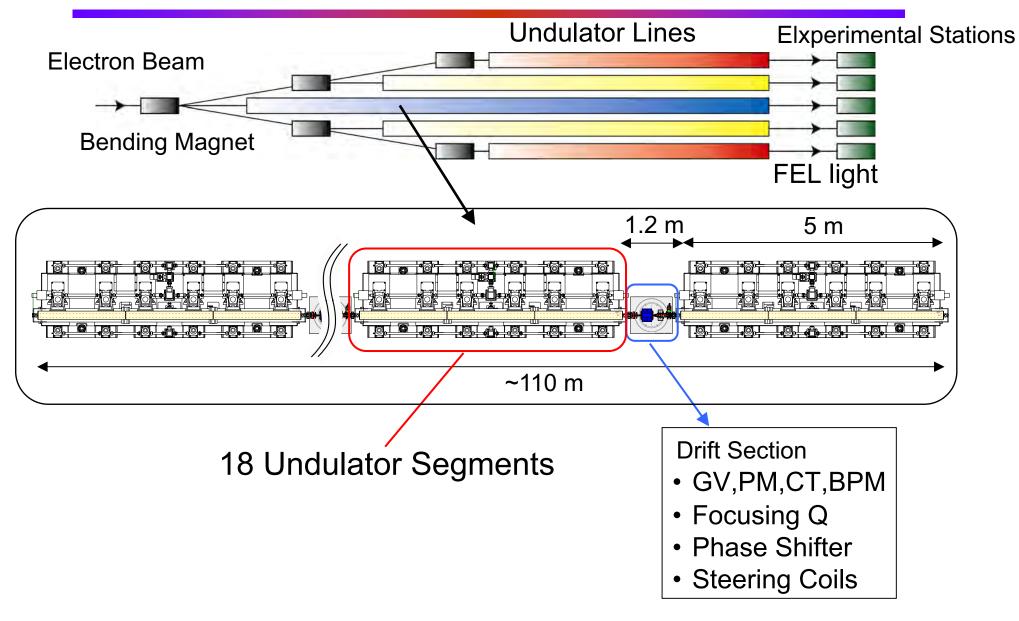
## **Beam Monitor Devices**

#### By Y. Otake team.





# **SP-8 XFEL Undulator Line**



Undulator is ready for mass production.

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

# **Undulator Parameter**

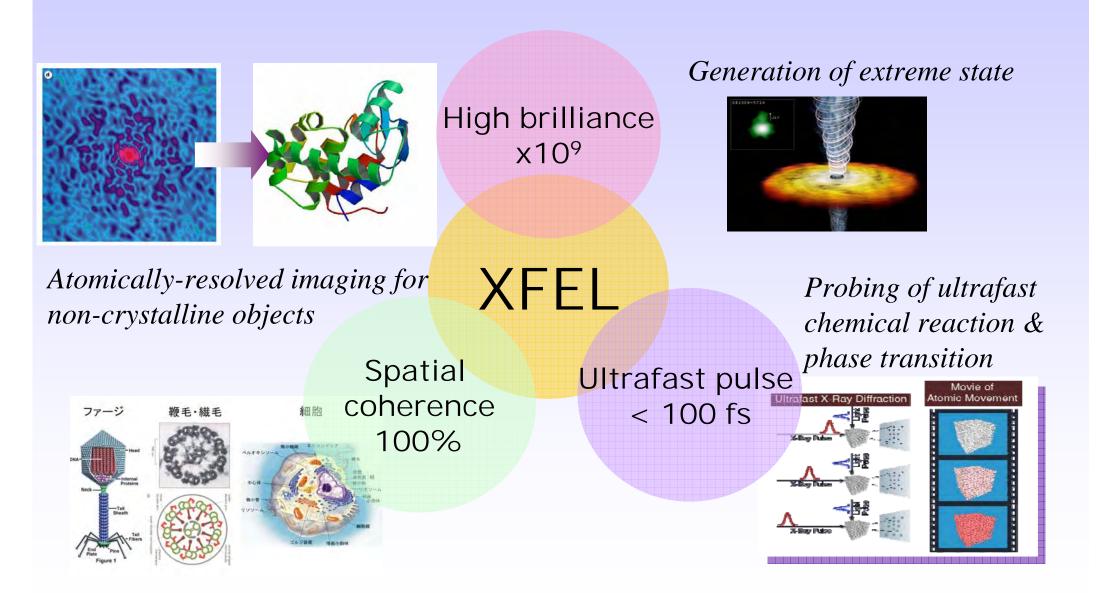
Undulator Type		In-Vacuum Planer Undulator
Active Length		5 m
Undulator Period		18 mm
Magnetic Circuit		Hybrid (NdFeB+Permendur)
Peak Field	Maximum	1.31 T
	Nominal	1.13 T
K	Maximum	2.2
	Nominal	1.9
Gap	Minimum	3.5 mm
	Nominal	4.5 mm
Maximum Attractive Force		~ 6 ton

### **Undulator for XFEL/SPring-8**

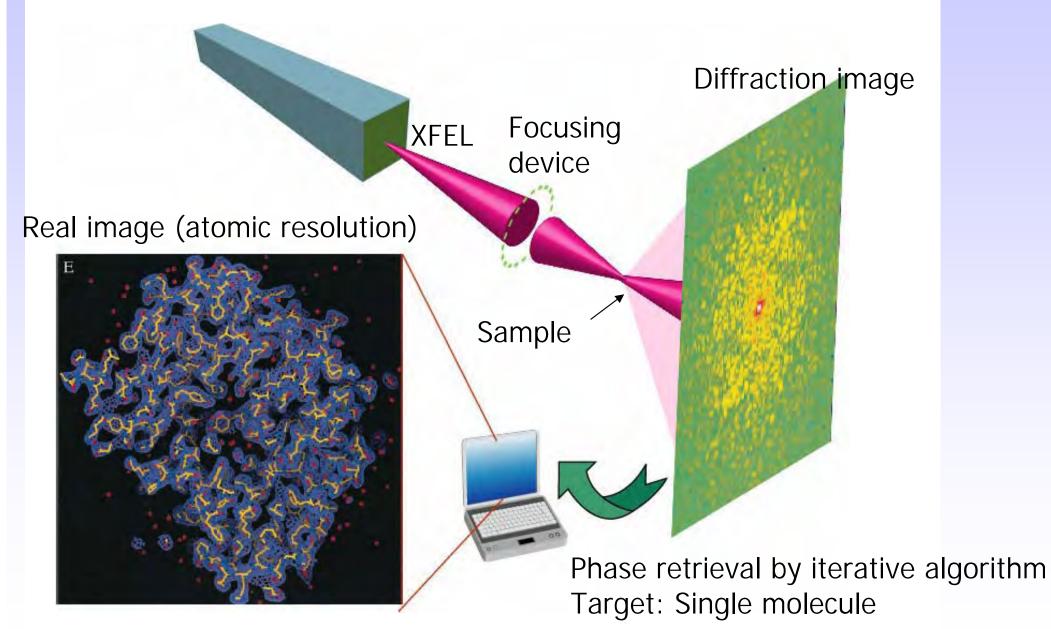
Outlook of 5 m long in-vacuum undulator for X-ray FEL.

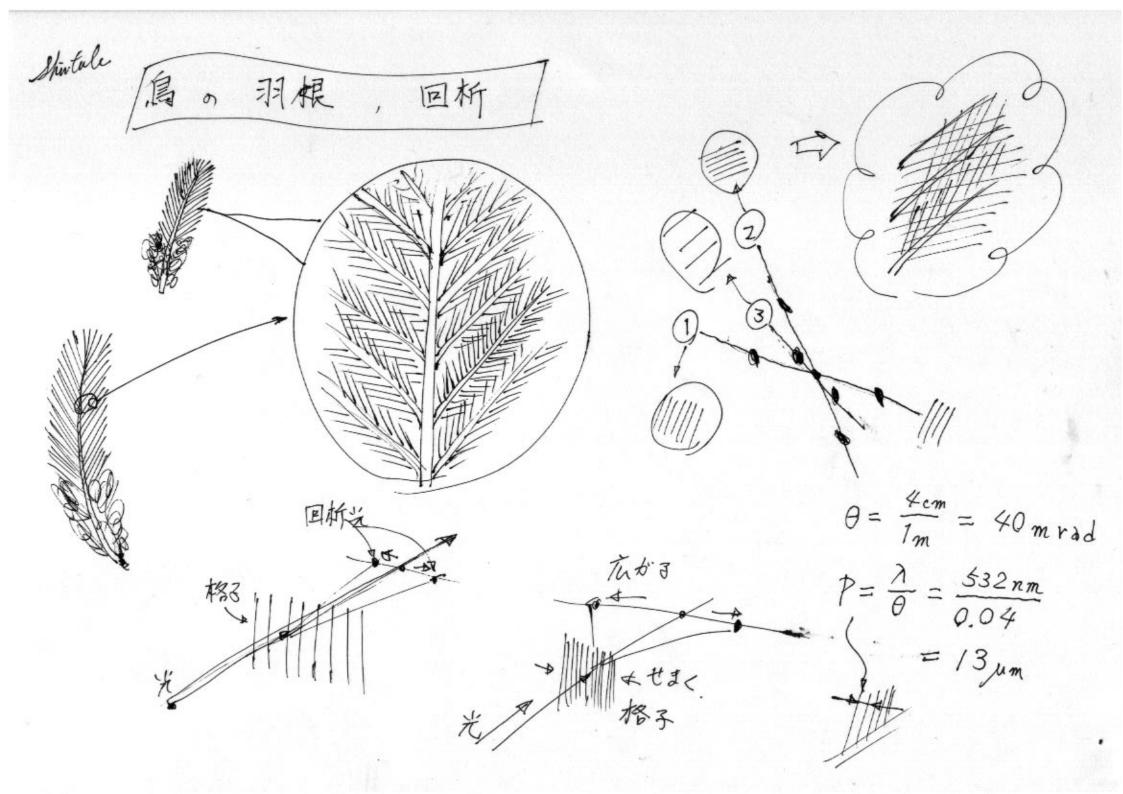
NeFeB magnet array, undulator period is 18 mm.

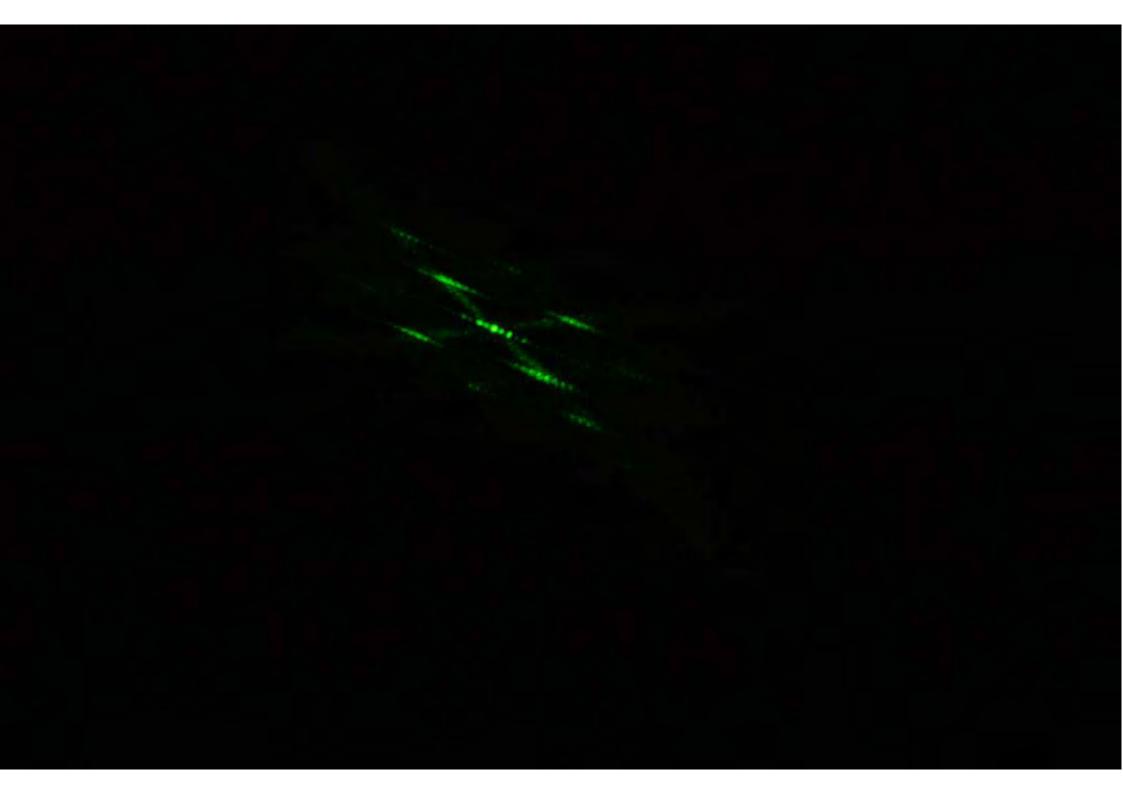
## **Science with X-ray Free Electron Laser**



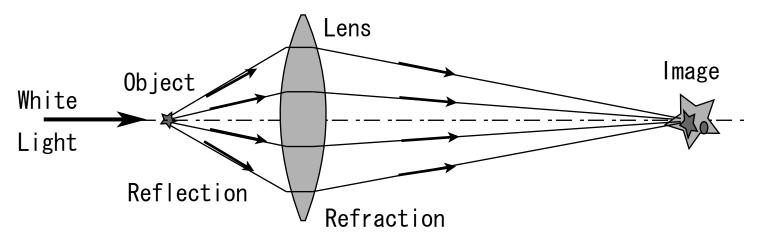
## **Coherent diffraction imaging**



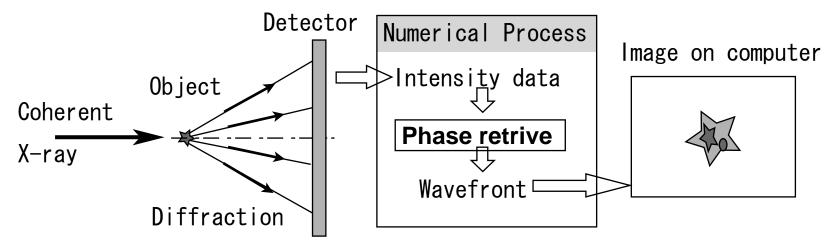




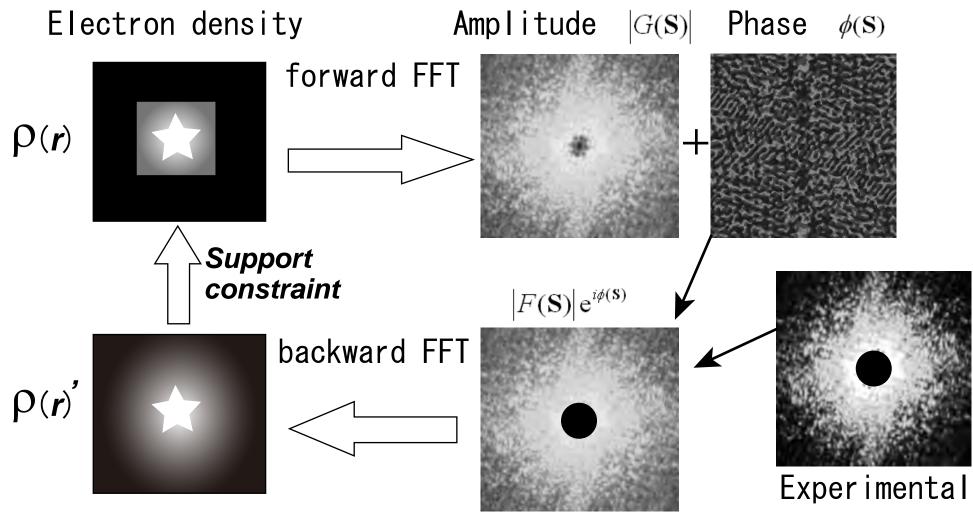
### **Optical Microscope**



### **Lensless Diffraction Microscope**

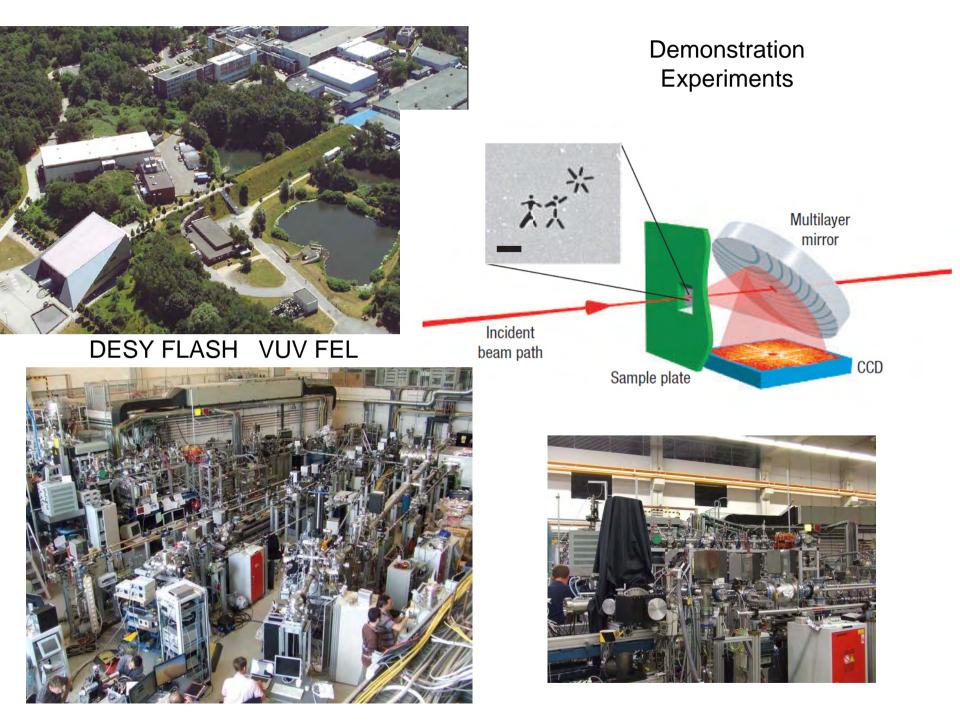


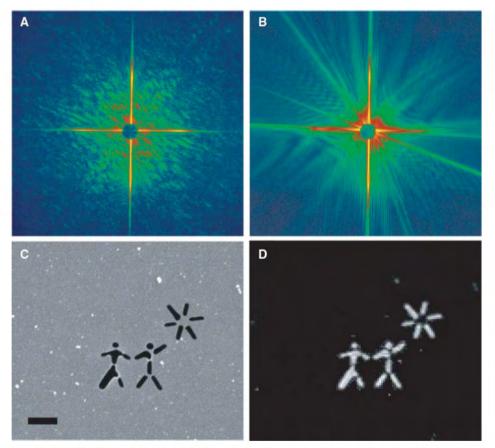
## **Iterative Phase Retrieval**



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

Data  $|F(\mathbf{S})|$ 





**Fig. 3.** (A) Diffraction pattern recorded with a single FEL pulse from a test object placed in the 20- $\mu$ m focus of the beam ( $\beta$ ). (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  $\mu$ 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

Tsumoru Shintake

RIKEN SPring-8 Center, Harima Institute, 1-1-1 Kouto, Sayo, Hyogo 679-5148, Japan (Received 23 April 2008; revised manuscript received 21 August 2008; published 3 October 2008)

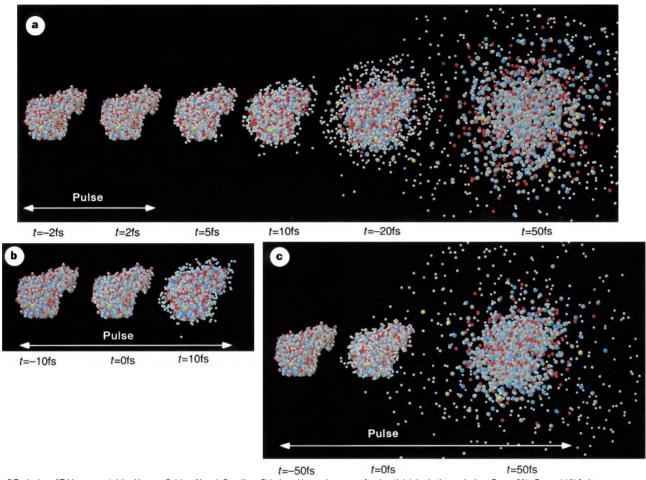
The number of photons produced by coherent x-ray scattering from a single biomolecule is very small because of its extremely small elastic-scattering cross section and low damage threshold. Even with a high x-ray flux of  $3 \times 10^{12}$  photons per 100-nm-diameter spot and an ultrashort pulse of 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

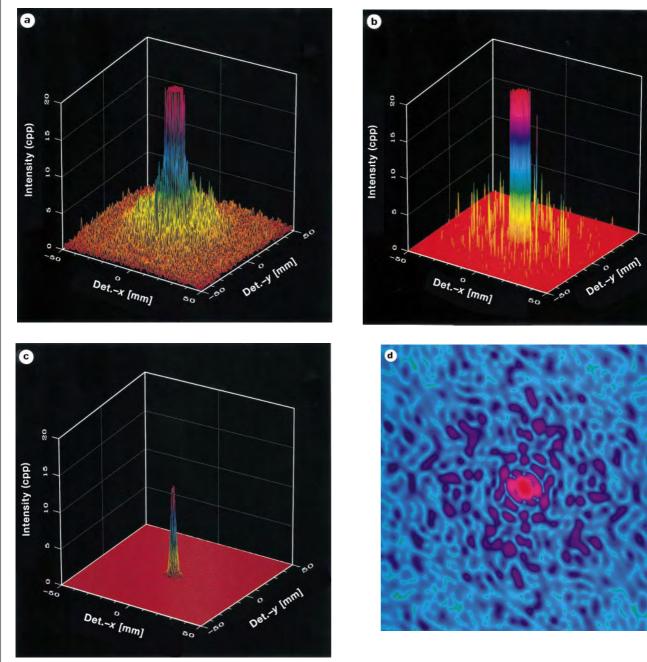
# Physical Origin of Difficulty

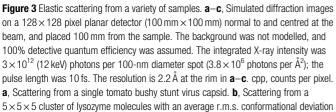
- In observations of scattered X-rays on a detector, the transfer of energy from wave to matter is accompanied by the quantization of the photon energy. Unfortunately, X-rays have a considerably high photon energy of 12 keV at wavelengths of 1 Å, which is required for atomic resolution imaging.
- Therefore,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



**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  $3 \times 10^{12}$  (12 keV) photons per 100-nm diameter spot ( $3.8 \times 10^6$  photons per Å<sup>2</sup>) 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.  $R_{\text{nucl}} = 7\%$ ,  $R_{\text{elec}} = 12\%$  **c**, Behaviour of the protein during an X-ray pulse with an FWHM of 50 fs.  $R_{\text{nucl}} = 26\%$ ,  $R_{\text{elec}} = 30\%$ .





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.

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### Single Biomolecule Imaging with XFEL

(Heterodyne Detection + Holographic Recording)

"Weak diffraction from biomolcule is amplified by 10 ~ 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

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

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

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

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

• Even if P<sub>2</sub> is 10<sup>-6</sup> times smaller, the signal is amplified to 10<sup>-3</sup> level. This is +30 dB amplification.

T. Shintake CAS School Brunnen 2-9 July 2003

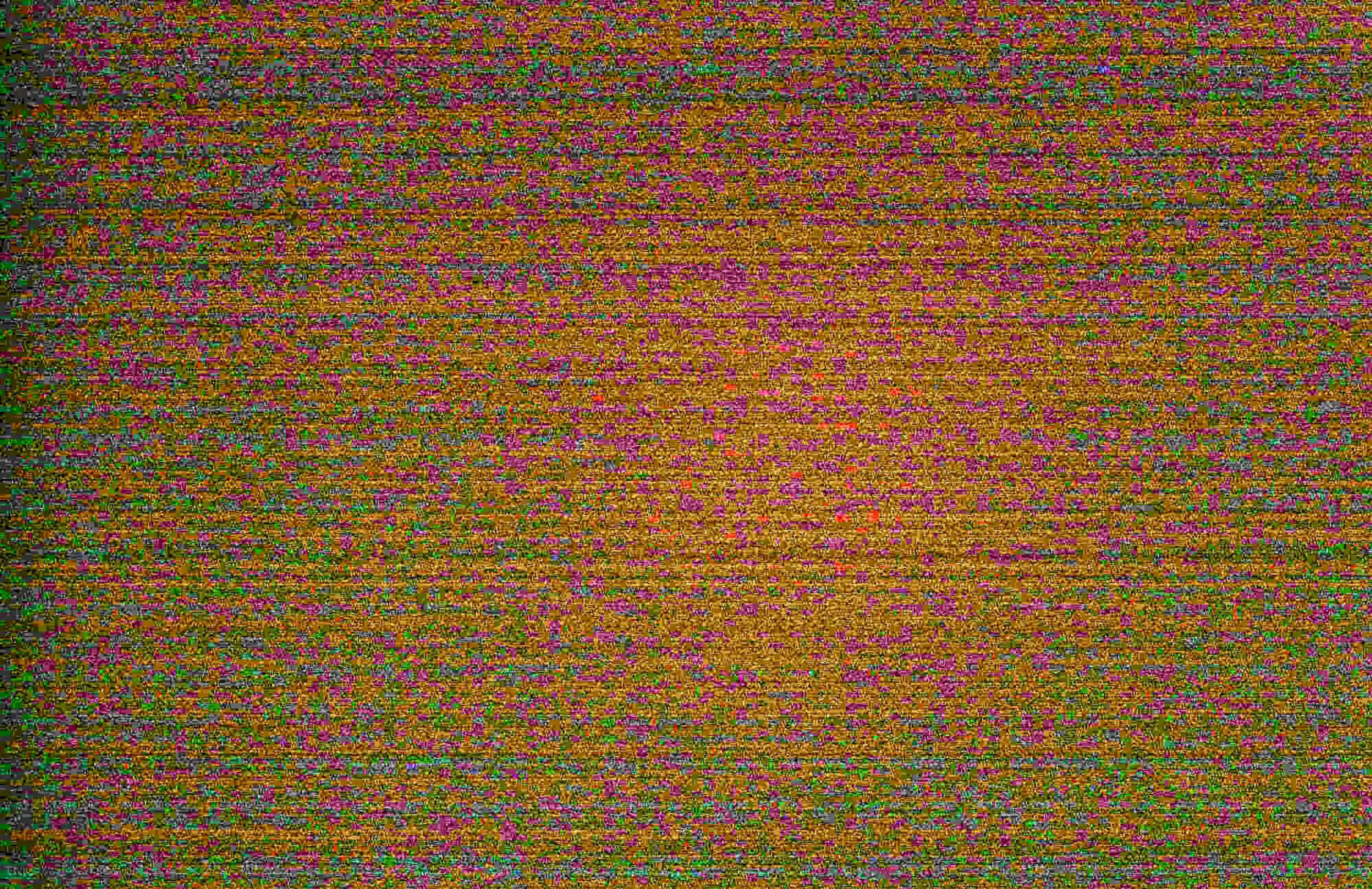
# Does noise increase or decrease?

- 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







#### TSUMORU SHINTAKE

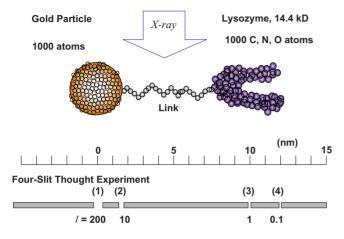


FIG. 4. (Color online) Conceptual diagram of a single lysozyme molecule linked to a gold particle (diameter of atoms is not drawn to scale). The gold particle produces 200 times more coherent x-ray scattering than the single lysozyme molecule. The bar at the bottom of the figure represents a four-slit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

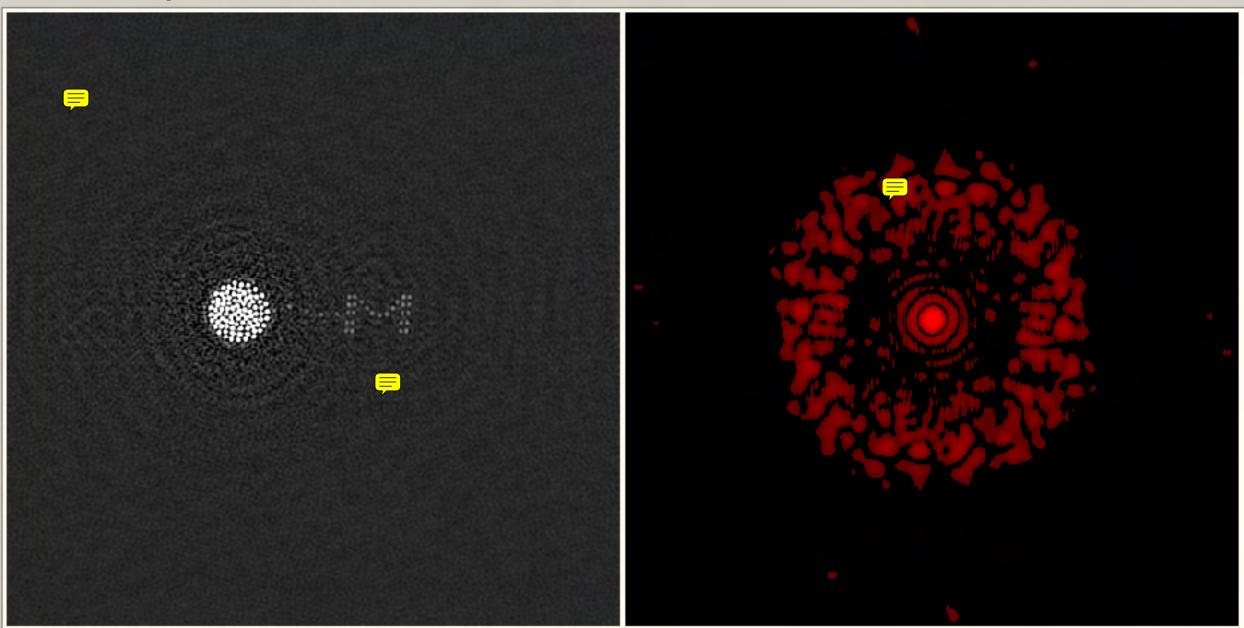
Fourier transform holography uses spherical waves as reference waves to record the phase of an object wave. The intensity of the reference wave is chosen such that it is comparable to that of the object wave to obtain the best contrast. To obtain better image quality, the size of the reference wave source 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

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

Here,  $I_i$  represents the flux from the *i*th slit,  $2\theta$  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.

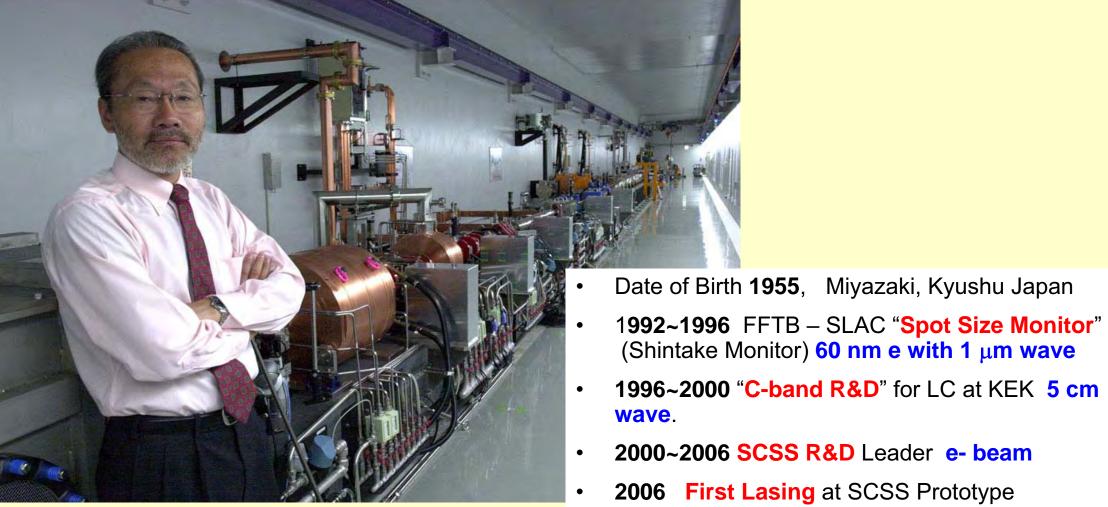
In Fig. 5(c), the curve at the bottom indicates the scattered wave from the biomolecule when it is directly observed without using the reference pump wave. It is a very weak signal with a relative intensity of approximately 1. In practice, the signal is quantized by the photon energy, leading to a loss 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

- Accelerator 49 nm wave
- 2006~ Now constructing 8 GeV XFEL/SPring-8 • for 0..1 nmm wave

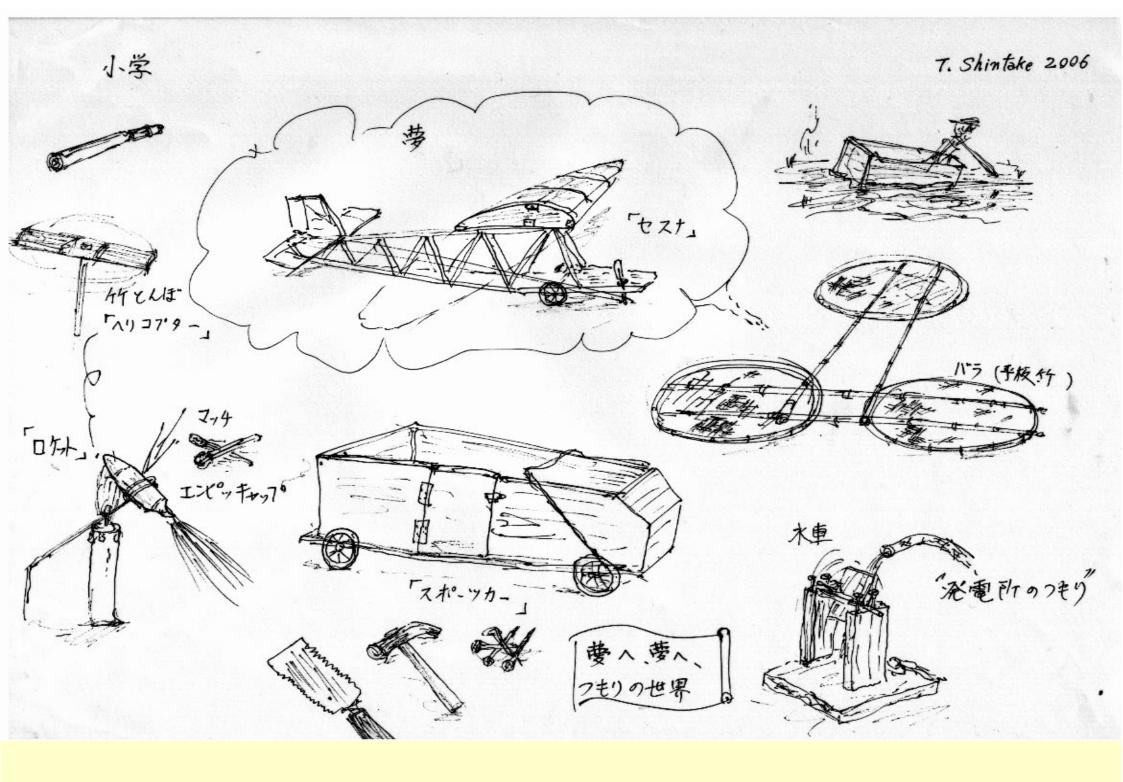


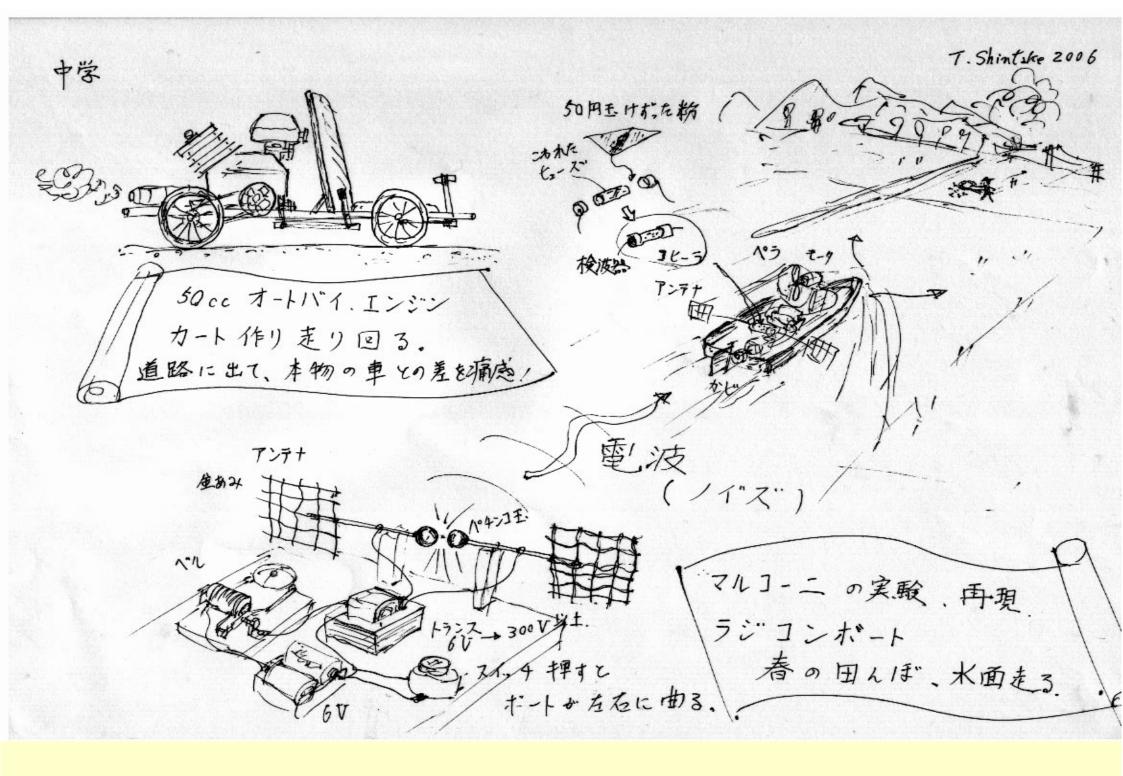
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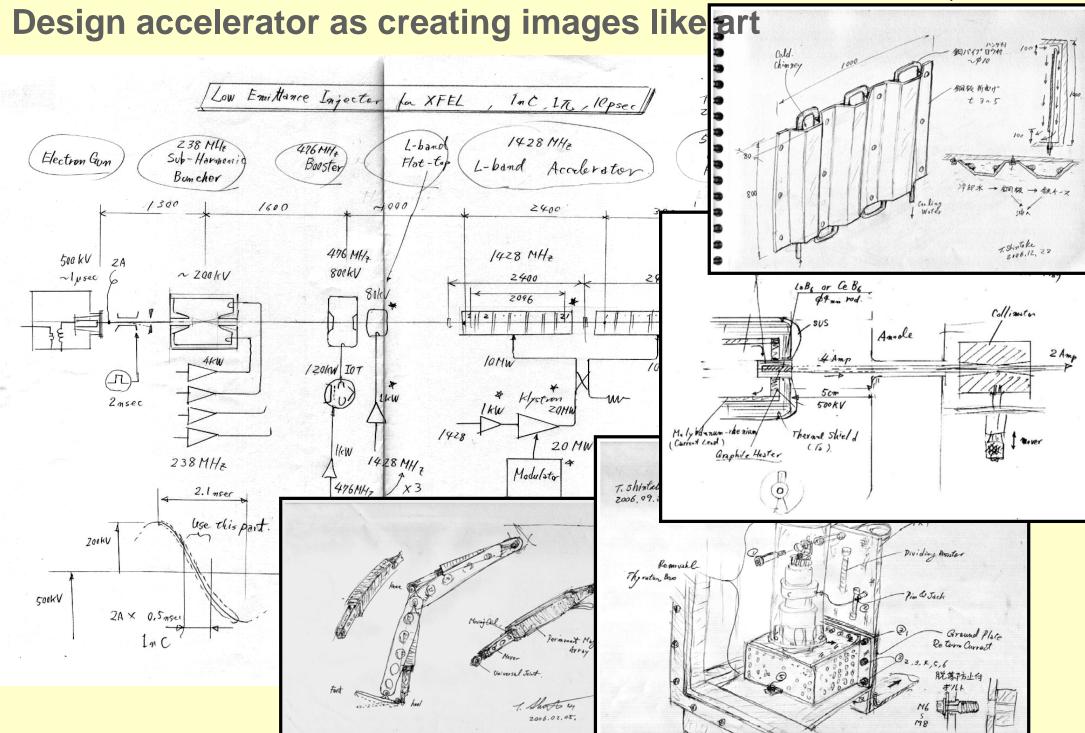
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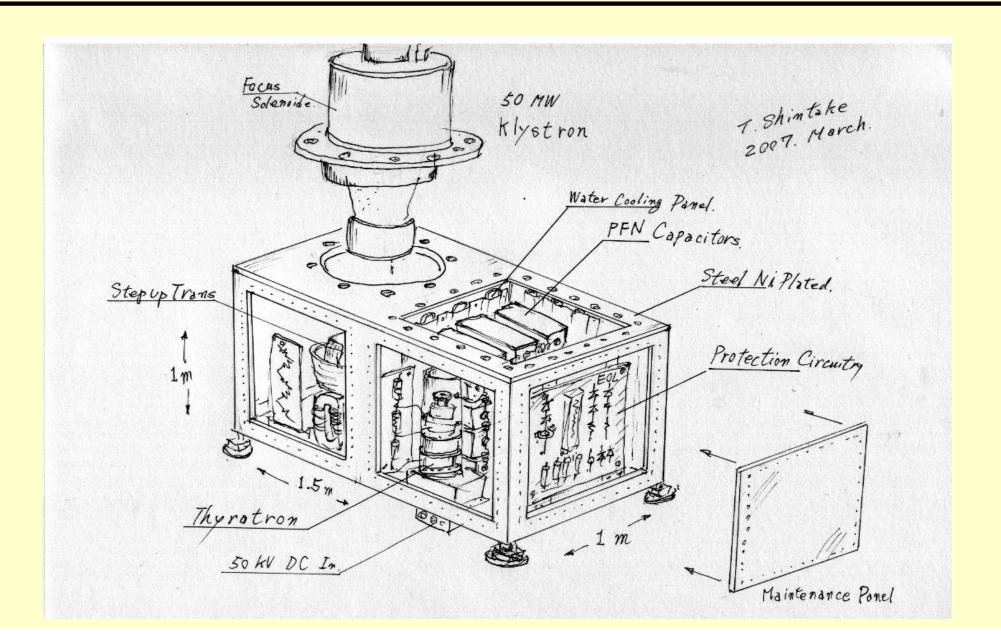
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#### Shintake, Summer 2008



Shintake, Summer 2008

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



### 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.