Beam Instrumentation for FE Lasers and Coherent X-ray Detection

Tsumoru Shintake
RIKEN/SPring-8

- News from Japan, XFEL project has been funded.
  - 290 MUSD, 5 year construction, beam commissioning will start in the year 2010.

- Technical Challenge for Precise Electron Beam Alignment in Undulator Line (a few micron-meter / 10 m)
  - Cavity BPM
  - Ceramic Stand

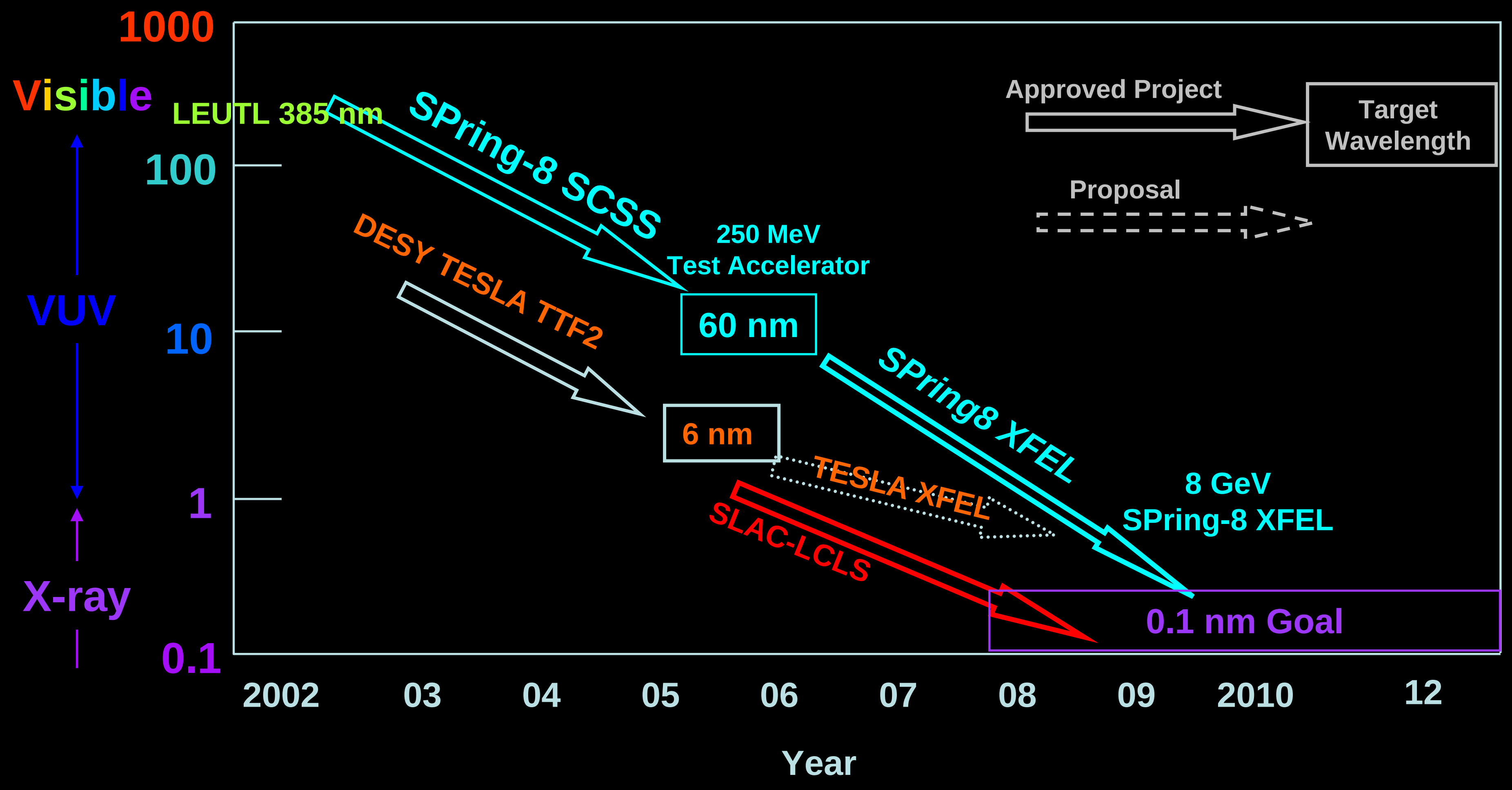
- *Possibility of Coherent X-ray Detection : New proposal*
  Protect Protein Crystal from damage under intense X-ray radiation.

News from Japan

- X-ray FEL project of RIKEN/SPring-8 has been funded.
  - Total budget ~ 290 M$ (375 OkuYen), including facility, linac, X-ray beam line, first experiment, excluding labor.
  - Construction: 2006-2010
  - Beam commissioning will start from 2010
  - Max e-beam energy: 8 GeV, total facility length < 700 m.
  - Max photon energy: 10 keV
  - Pulse format: 60 pps,
  - single bunch mode (0.3 nC, 100 fsec, 2 GW)
  - multi-bunch mode (2.6 nsec, 0.1 nC x 100 bunches, <0.1 GW)

- Test Accelerator has been constructed at RIKEN/SPring-8.
  - Construction: 2005
  - Beam commissioning 2005, Nov ~ 100 nm, Spontaneous
  - Several hardware and software errors were found, now under upgrade, and repair.
  - FEL commissioning in 2006, June.

Milestone of SPring-8 X-FEL



SCSS & X-ray FEL Beam Parameter

at undulator section

		Test Accelerator	X-ray FEL	
Beam Energy	E	0.25	6.0	GeV
X-ray Wavelength	λ	60	0.1	nm
Beam Emittance (slice)	ε_n	1	0.85	πmm.mrad
Bunch Length	Δz	150	24	µm
	FWMH	500	80	fs
Peak Current	I_p	0.3	3	kA
Charge per bunch	q	0.2	0.4	nC
FEL Saturation Length	L_{sat}	8.5	80	m
Undulator Parameter	λ_u	15	15	mm
	K	1.3	1.3	
Length	L	9	100	m
Peak Brilliance		8 x 10^{27}	1 x 10^{33}	N/mm^2/mrad^2/0.1%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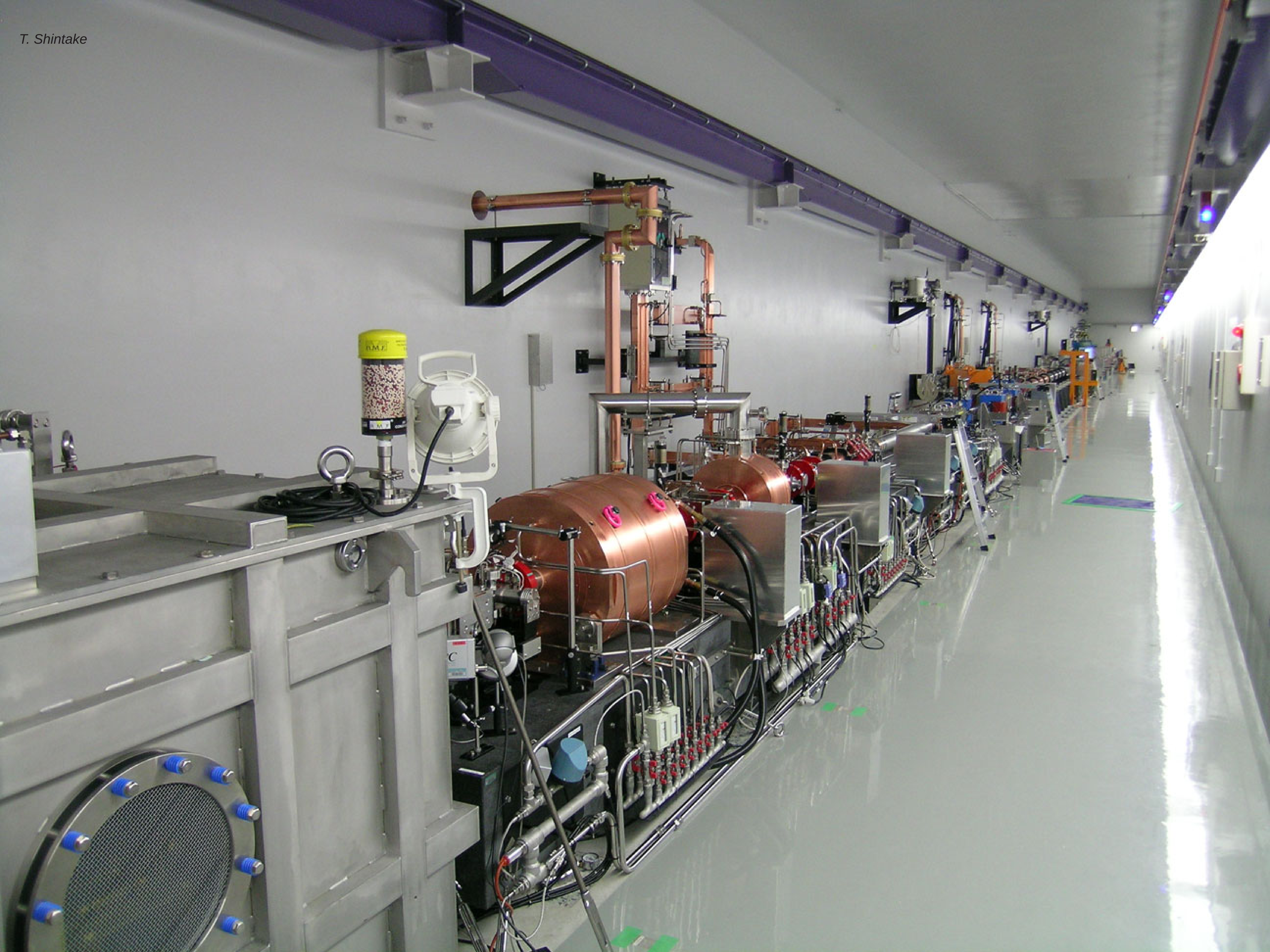
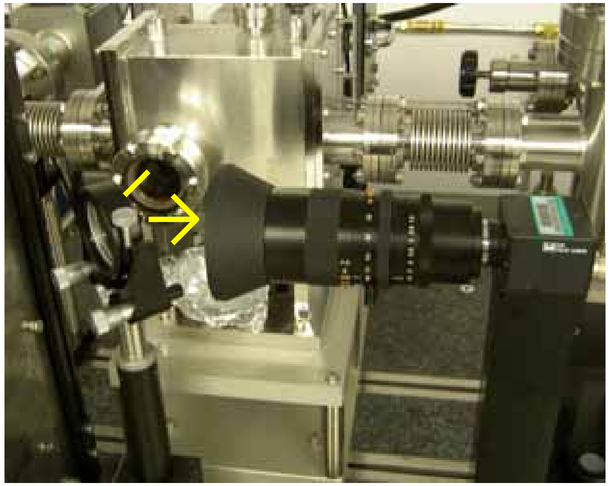
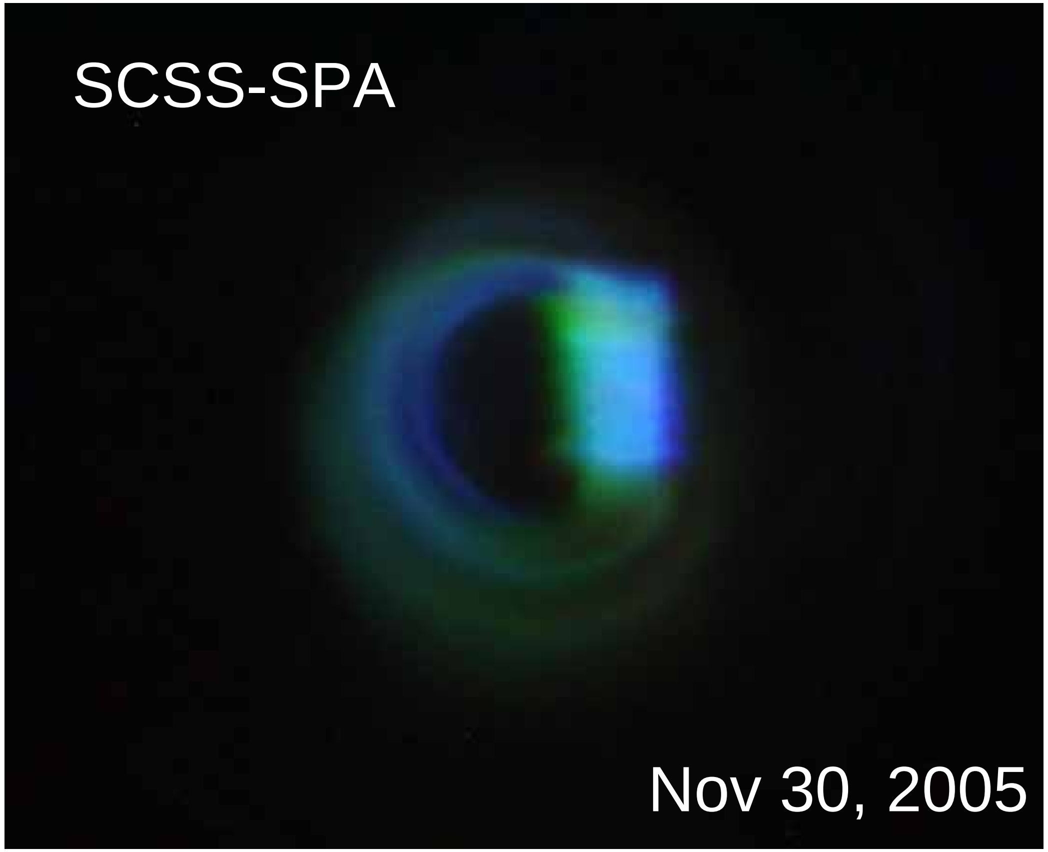


First beam





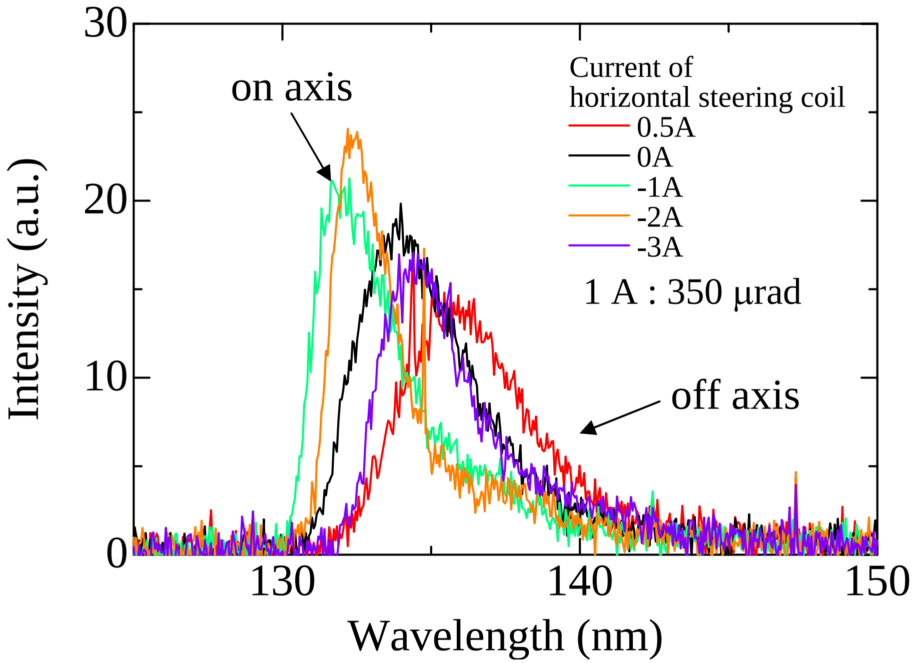
SCSS-SPA

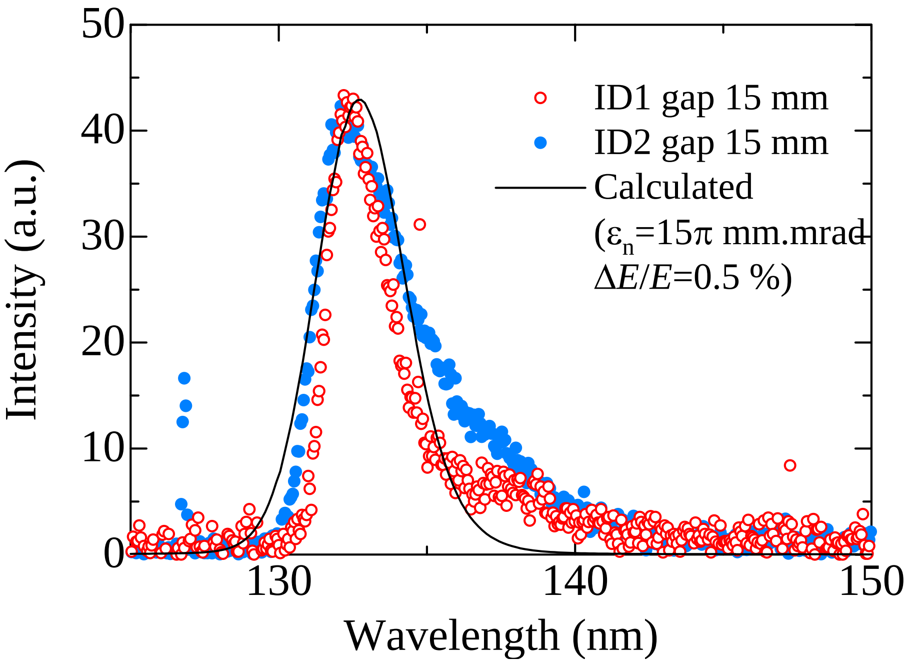
Nov 30, 2005

E_b=66 MeV, ID gap = 10 mm, λ= 480 nm

Energy Spectrum of Spontaneous Radiation

by M. Yabashi et al.





Spectrum response to horizontal deflection of e-beam

E_b=122 MeV

ID1 gap =15 mm

Incident Slit Aperture = 1 mm (H)

On-axis Spectrum

Integrated with 1000 shots

E_b=122 MeV

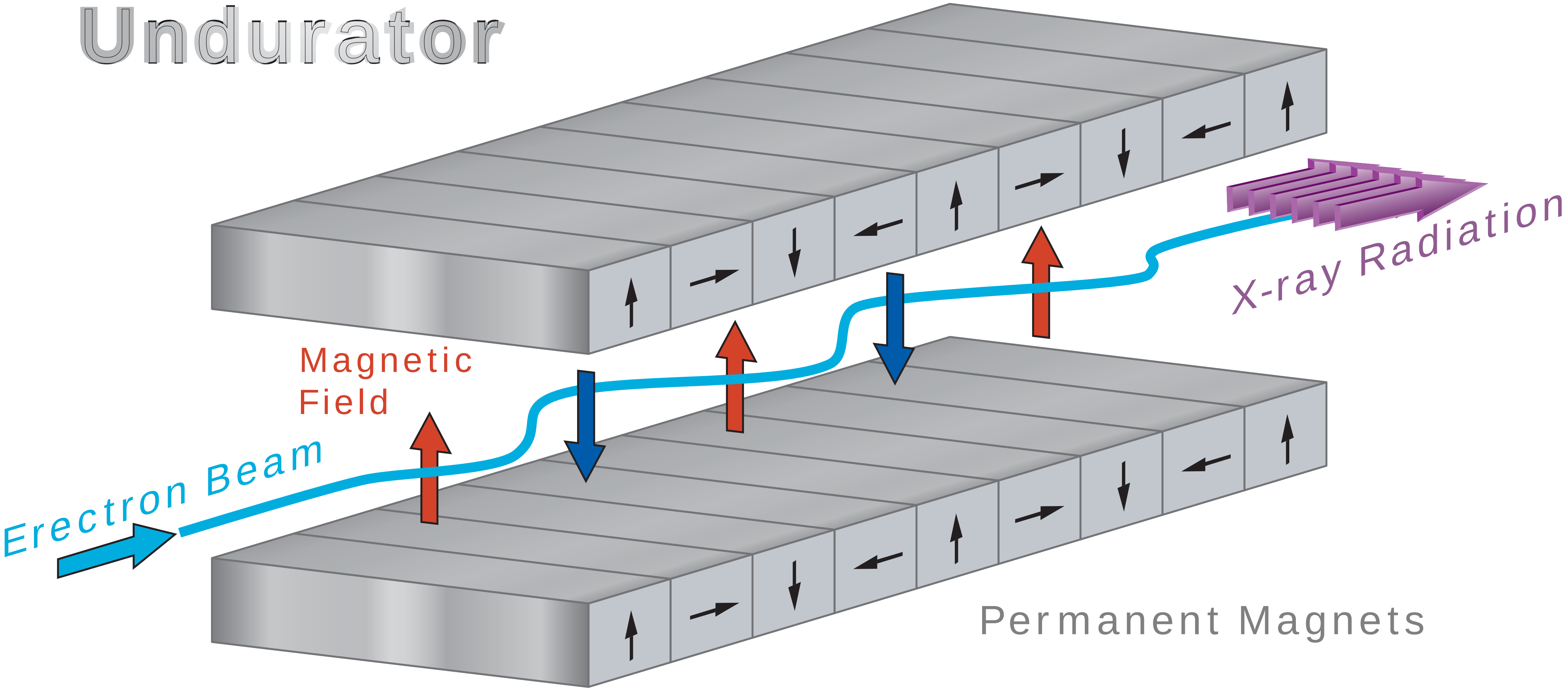
Incident Slit Aperture = 1 mm(H)

Measured Bandwidth (FWHM)

ID1: 1.8 %, ID2: 2.8 %

Undurator

T. Shintake



http://www-xfel.spring8.or.jp

SPring-8 Compact SASE Source

021653

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For SCSS Staff

What's NEW!!

10 May 2005: SCSS conceptual design report has been released. Click here to download (6.7MB).

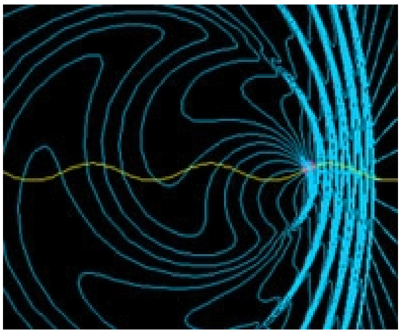
Welcome to SCSS Home

SCSS is an abbreviation for the SPring-8 Compact SASE Source, and is a high peak-brilliance soft X-ray free electron laser project for R&D aiming at realization of an angstrom X-ray laser facility. SCSS will provide six order of magnitude peak-brilliance enhancement compared to the current third-generation sources at 3 ~ 20 nm range.

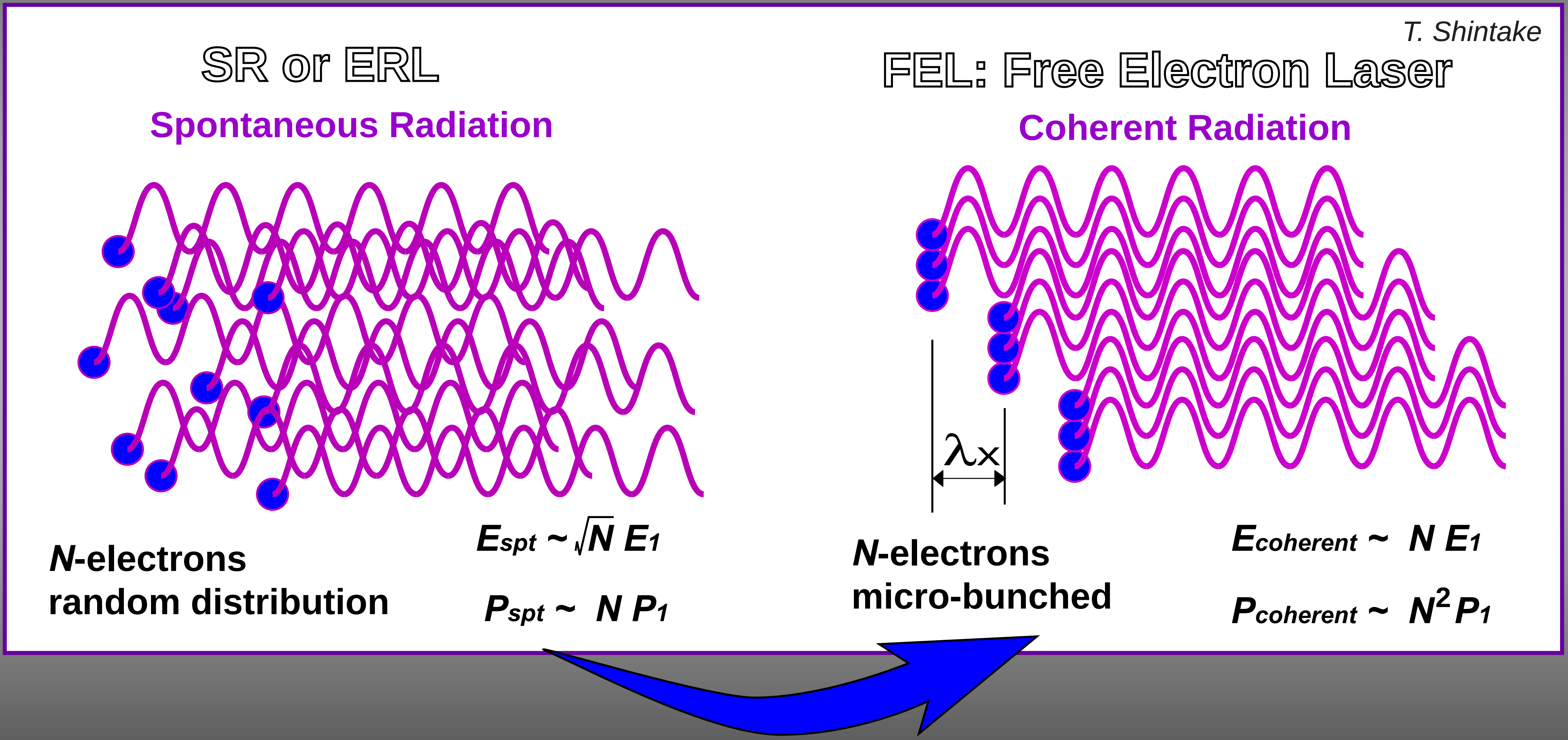
Radiation Simulator

Real-time radiation simulator for Windows. To download, click right image and fill your information for the future announce. It is just single executable file: Radiation2D.exe. To run, double click. Grab the center electron, and try to move it. You will see radiation. Chose circle trajectory from Setup Menu, you will see synchrotron radiation.
Note:Linux and Mac version are also available!!

25/Jul/2003 The Radiation2D Ver. 2.0 for Windows was released.



From SR to FEL



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SR or ERL

Spontaneous Radiation

***N*-electrons**
random distribution

$E_{spt} \sim \sqrt{N}\, E_1$

$P_{spt} \sim N\, P_1$

FEL: Free Electron Laser

Coherent Radiation

***N*-electrons**
micro-bunched

$E_{coherent} \sim N\, E_1$

$P_{coherent} \sim N^2 P_1$

Optical Power Enhancement

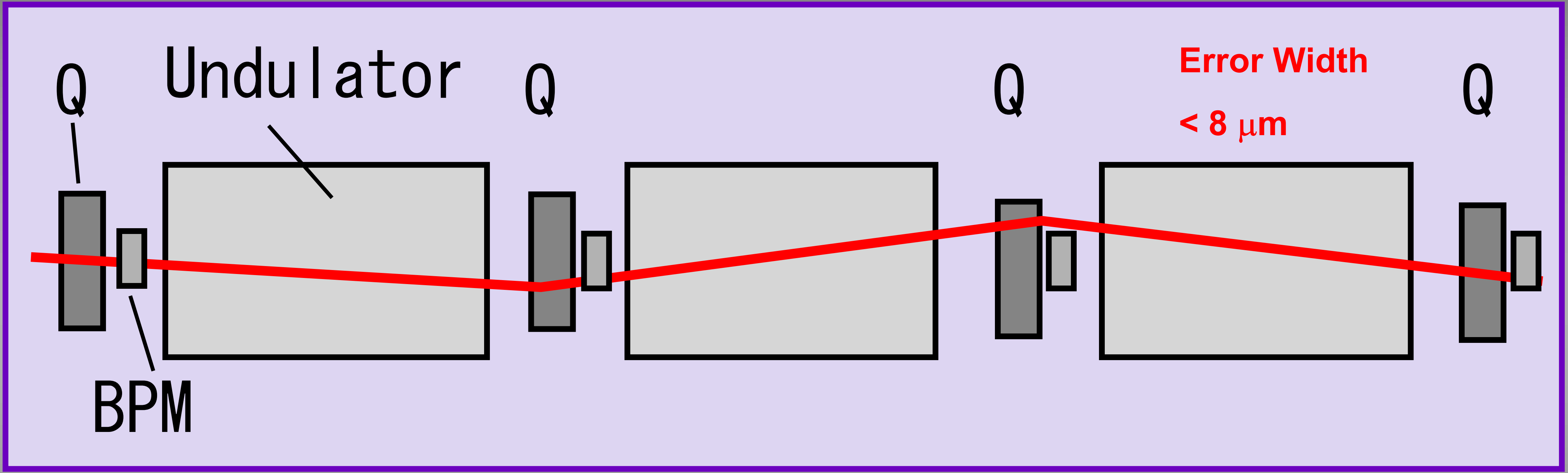
x $10^5 \sim 10^8$

Alignment Strategy

Presented by T. Shintake

- Beam trajectory in the undulator line has to be kept very straight to keep overlap e-beam with X-ray beam in order to obtain high FEL gain.
- Assume, undulator field in each segment (4.5 m long) is well tuned.
  - in situ field measurement tool will be R&D issue.
- Error sources (localized at segment-to-segment, beam focusing Q)
  - Alignment error of focusing Q-magnet, and wrong steering field.
  - End field error of undulator.
  - Residual field around beam line: magnetized material.
  - Earth magnetic field will be cancelled with long correction coil.
- Zig-zag error amplitude limit is only $|\Delta_{x,y}| < 4\ \mu\text{m}$.

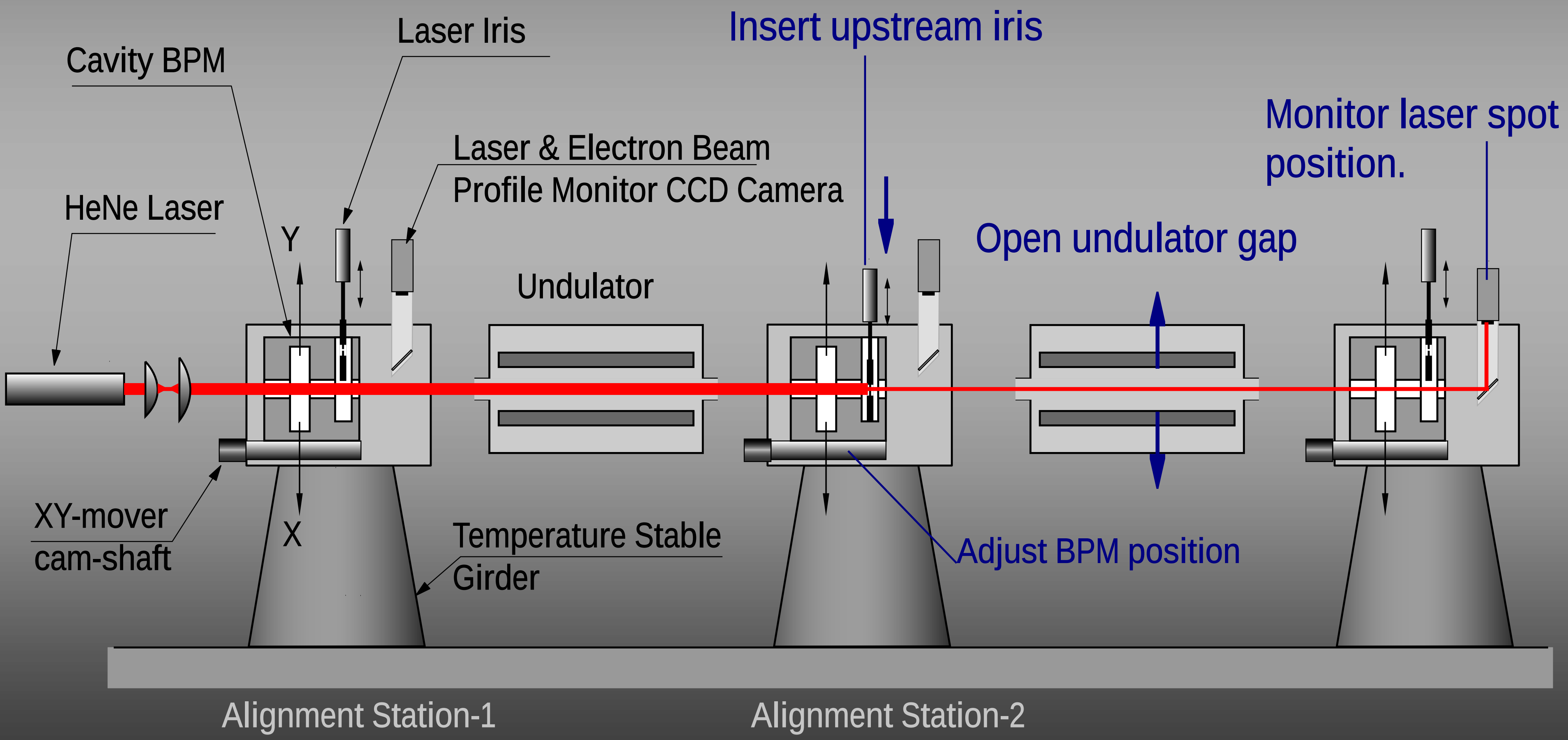
Electron Beam Trajectory Error Model



Q-magnet position error and field error at undulator matching section create beam trajectory error: zig-zag shape. Beam runs fairly straight line in each undulator.

BPM Alignment System for SASE FEL

T. Shintake



Insert upstream iris

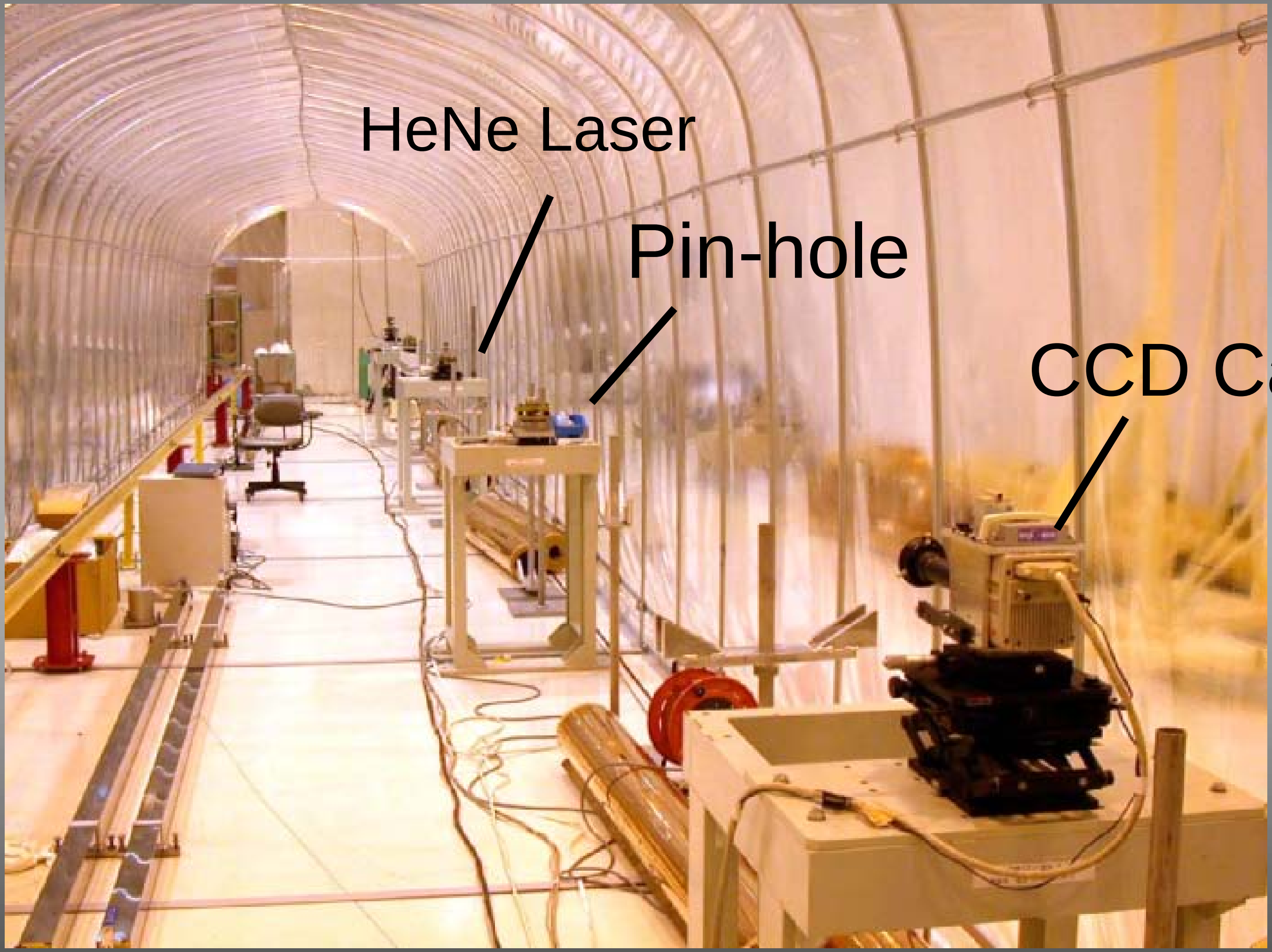
Monitor laser spot position.

Open undulator gap

Adjust BPM position

Laser Alignment Test in Air

by S. Matsui,
and Zhang Chao

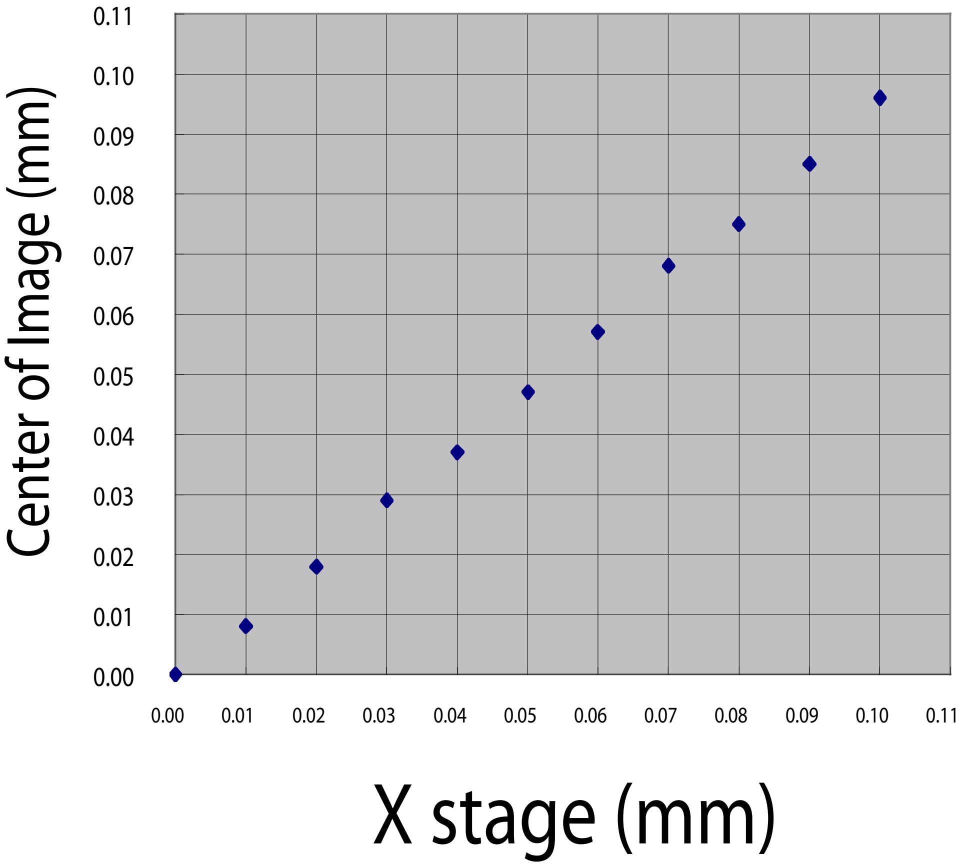


Distance from HeNe-laser to CCD : 20 m
Move pin-hople position
Readout laser-spot position on CCD.

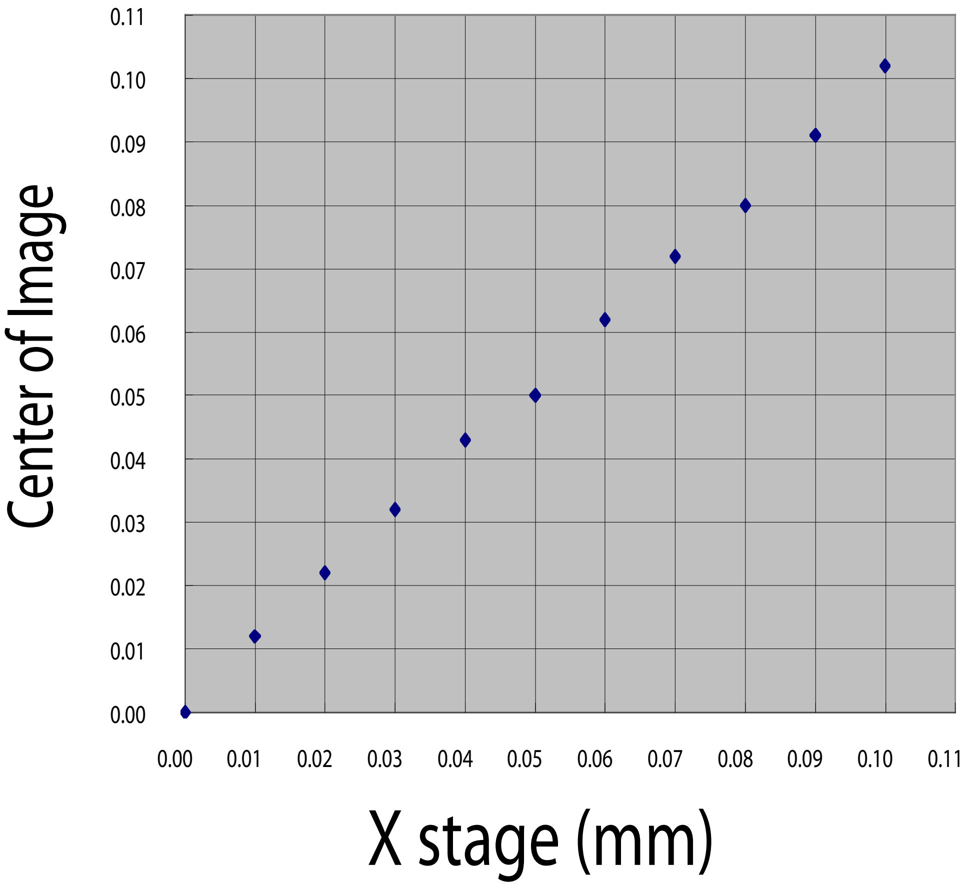
Alignment Test Result

2003.6.17

Iris at 10m



Iris at 15m

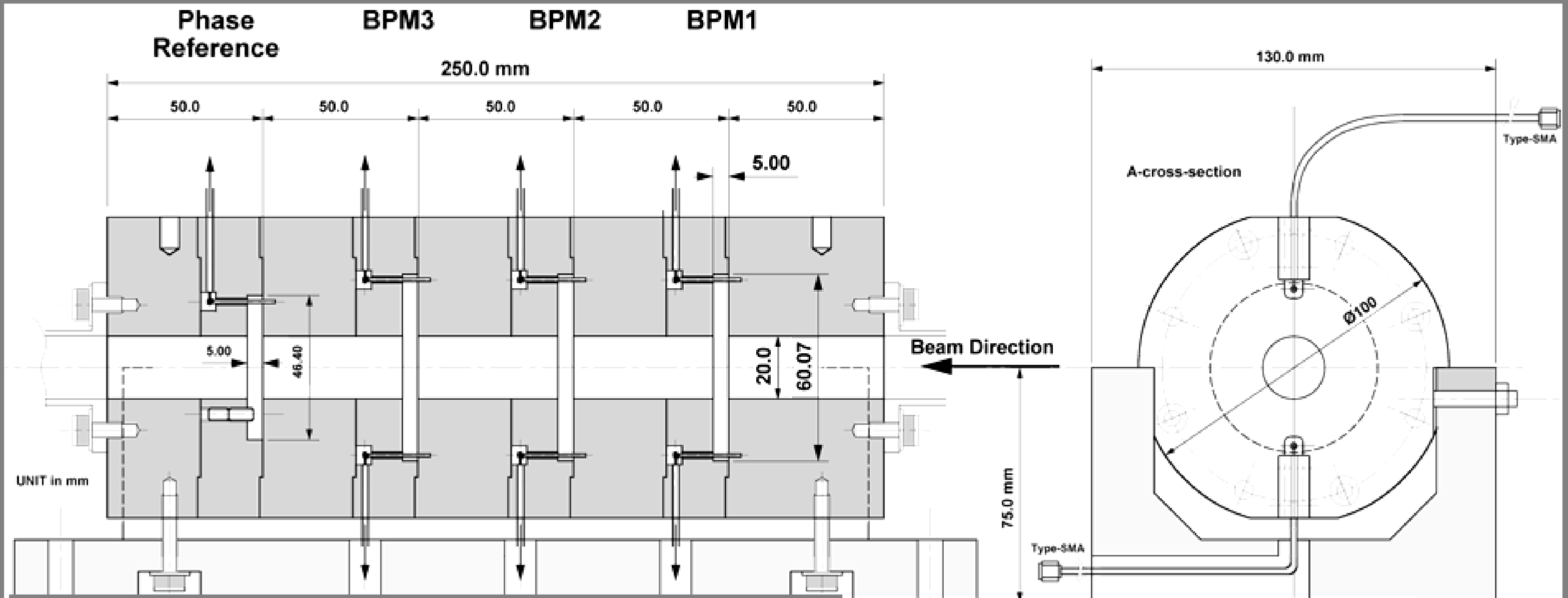


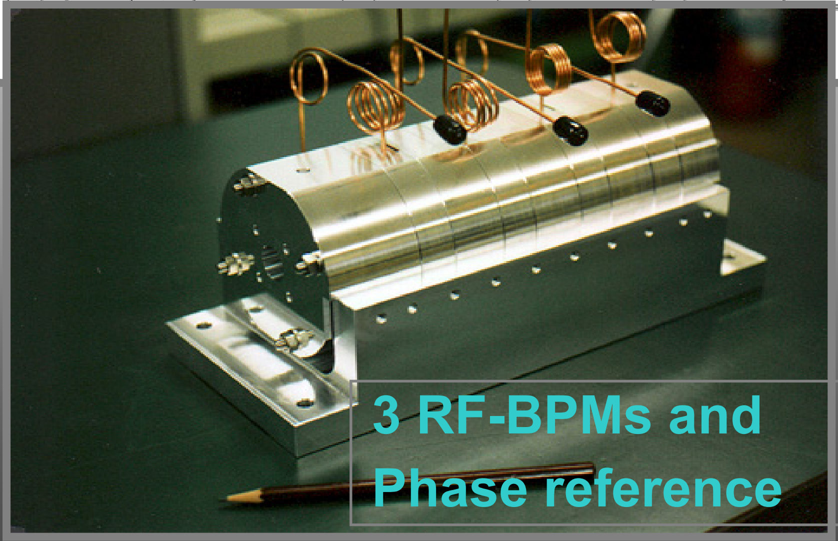
Averaging 10 frames on CCD,pixel mean center was determined.

Before XFEL

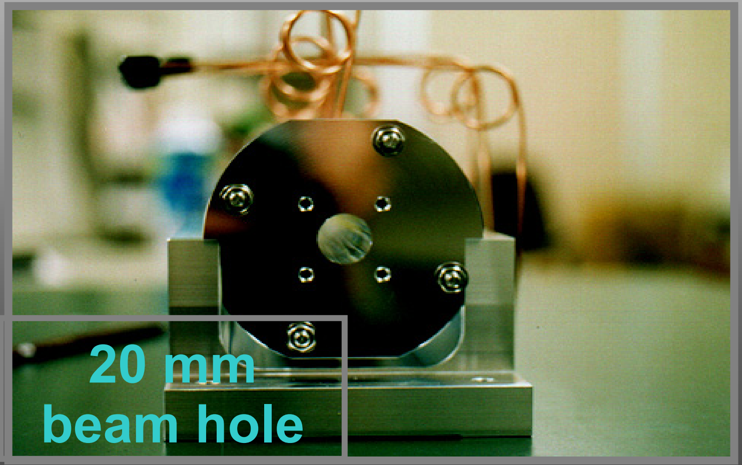
RF-BPM tested at FFTB

1995 T. Shintake, T. Slaton





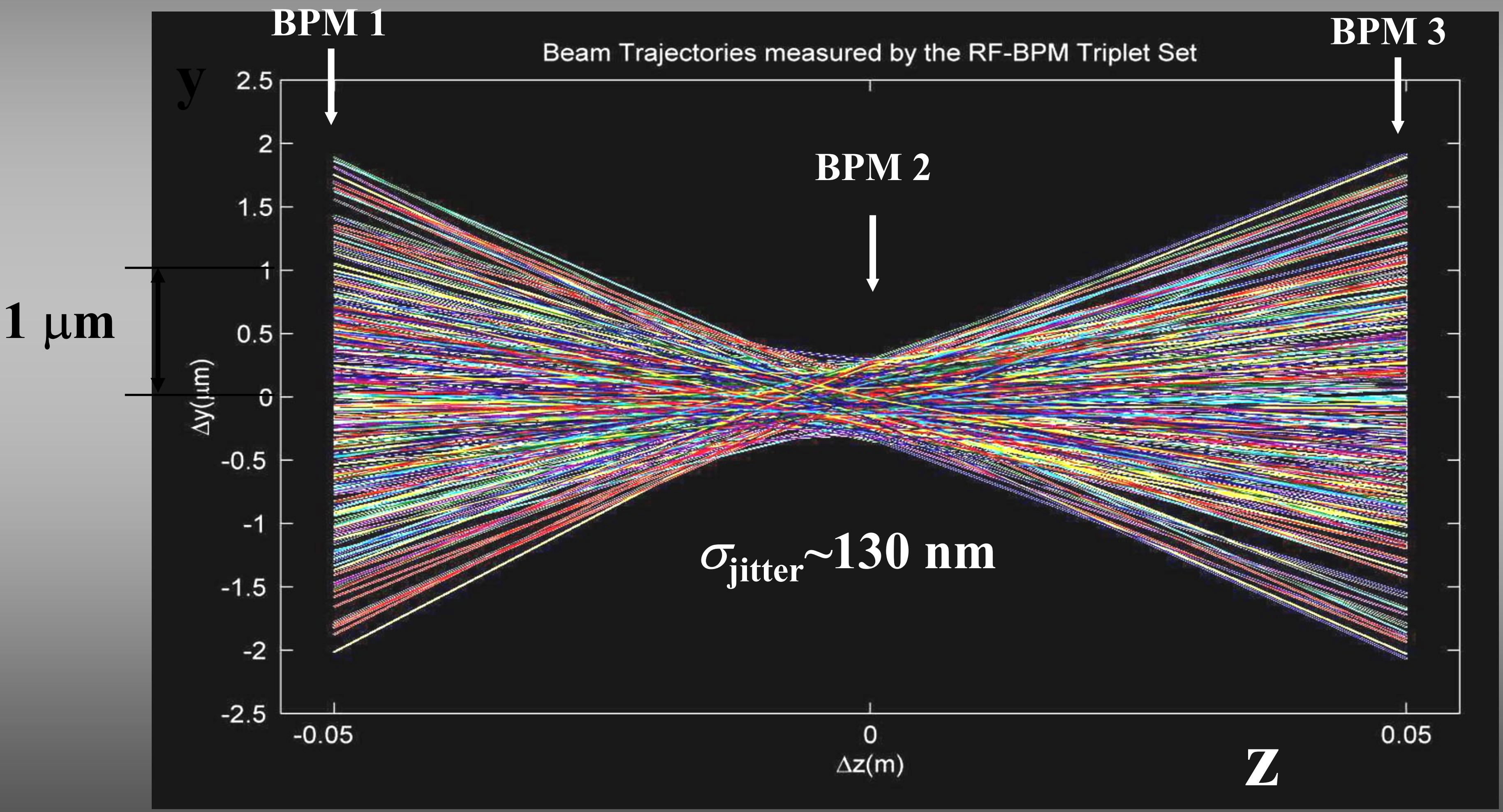
3 RF-BPMs and Phase reference



20 mm beam hole

Before XFEL

FFTB Measured Beam Trajectory



FFTB Test Results

BPM Resolution

$$\sigma_{bpm} = \sqrt{\frac{2}{3}}\sigma_{residual} \; .$$

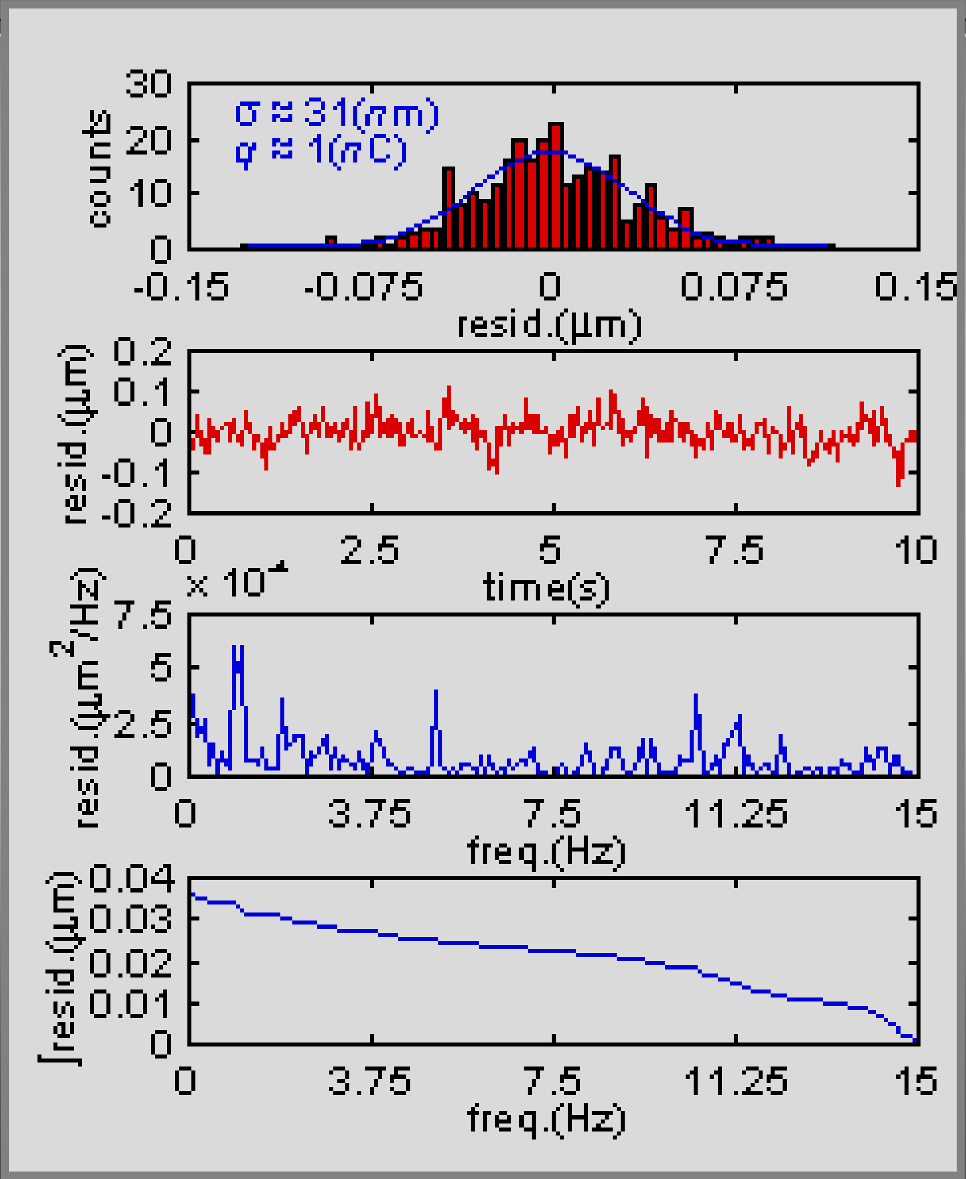
= 25 nm

Histogram

Time Structure

Frequency Spectrum

Frequency Integral



Cavity-BPM (Beam Position Monitor)

Newly developed Cavity-BPM
For SPring-8 XFEL. 4.7 GHz.

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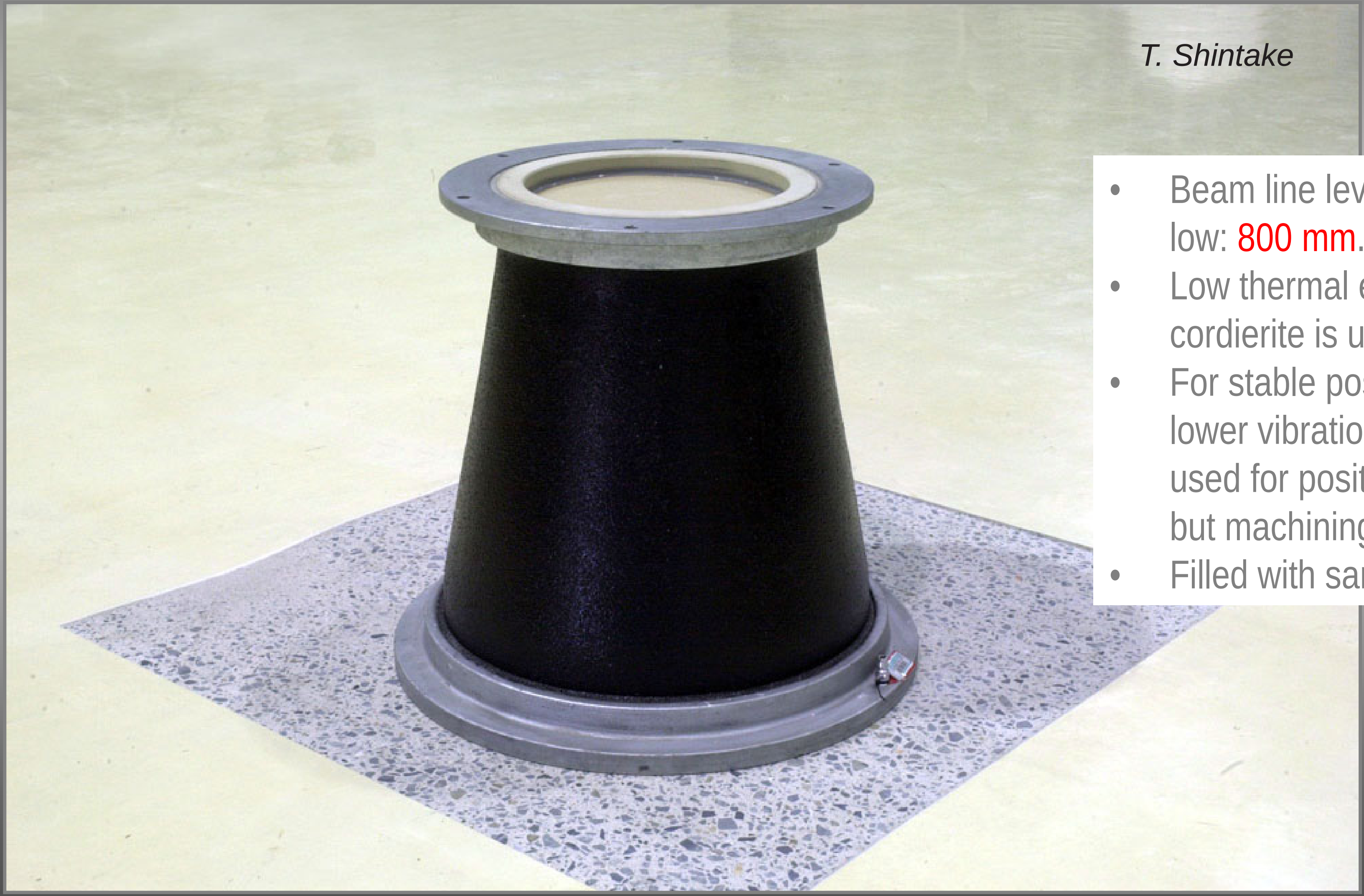
- TM110 mode excitation amplitude provides very linear beam position information.
- Slot-coupling design isolates TM110 BPM signal from TM010 common-mode mixing, which cause position offset.
- Electrical center meets very accurately with mechanical center in a few micron-meter (insensitive to variation of cable length, or detection circuit details).

Stable Support using Cordierite Ceramic



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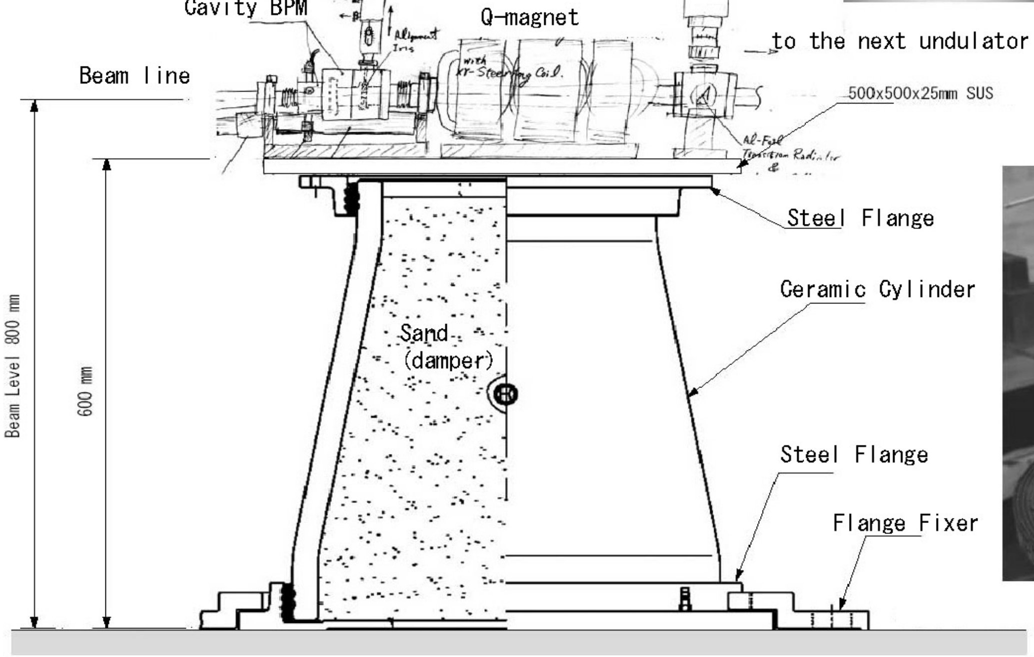
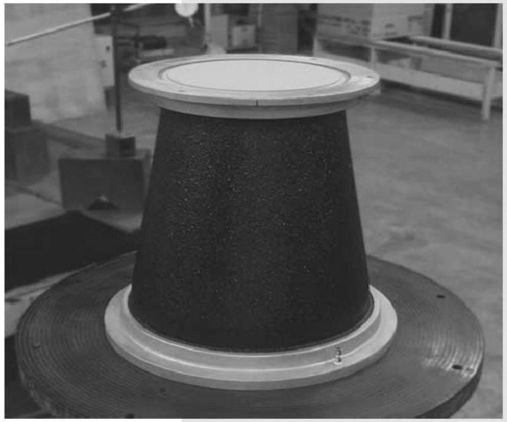
- Beam line level is designed low: 800 mm.
- Low thermal expansion cordierite is used.
- For stable positioning and lower vibration, No screw is used for position adjustment, but machining the spacer.
- Filled with sand for damper.

Stable Support using Cordierite Ceramic-2

Cordielite Ceramic
before sintering

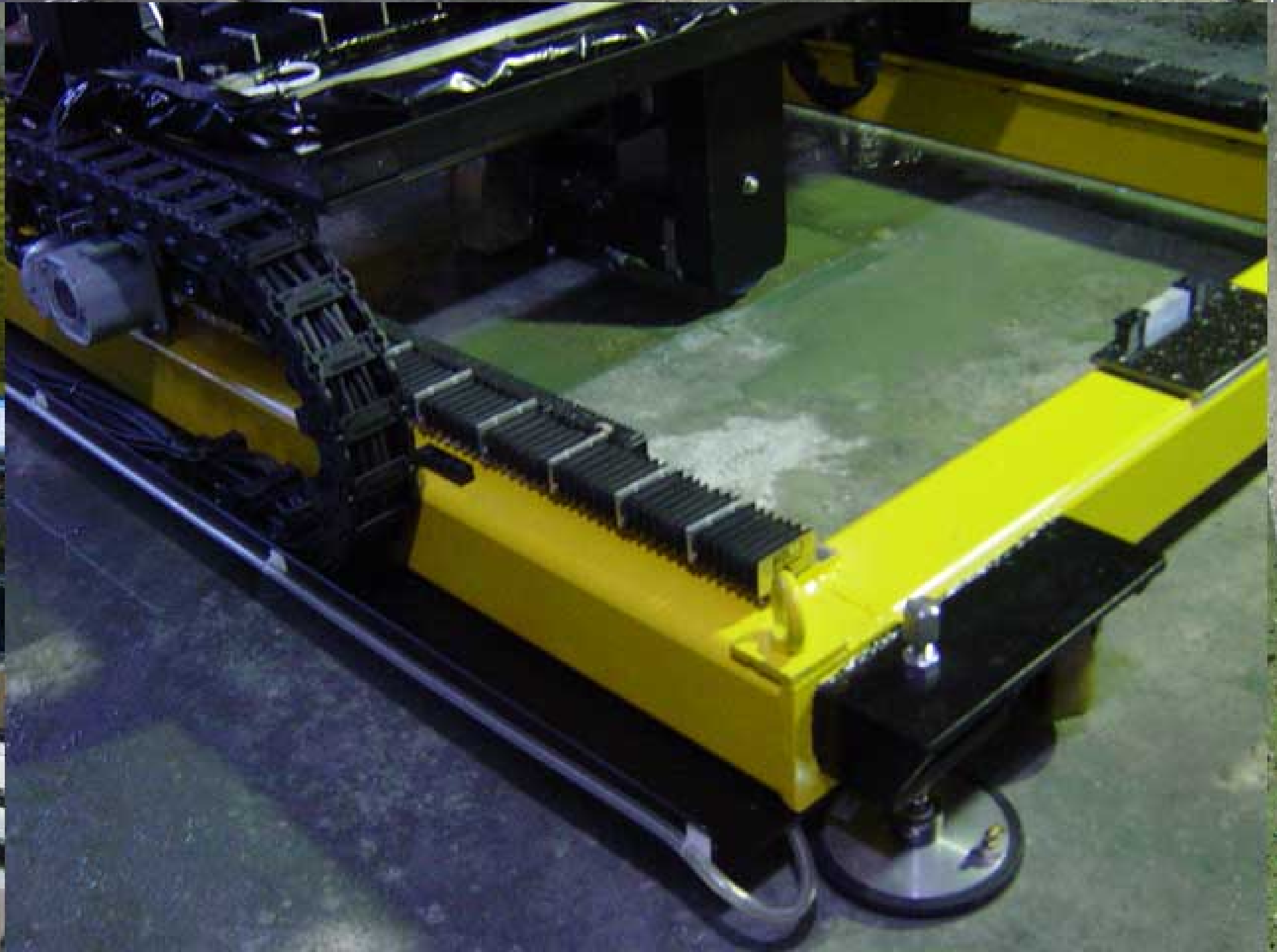




Ceramic Support using
Cordielite Ceramic


コンクリート床面研削装置
電源
研削画面

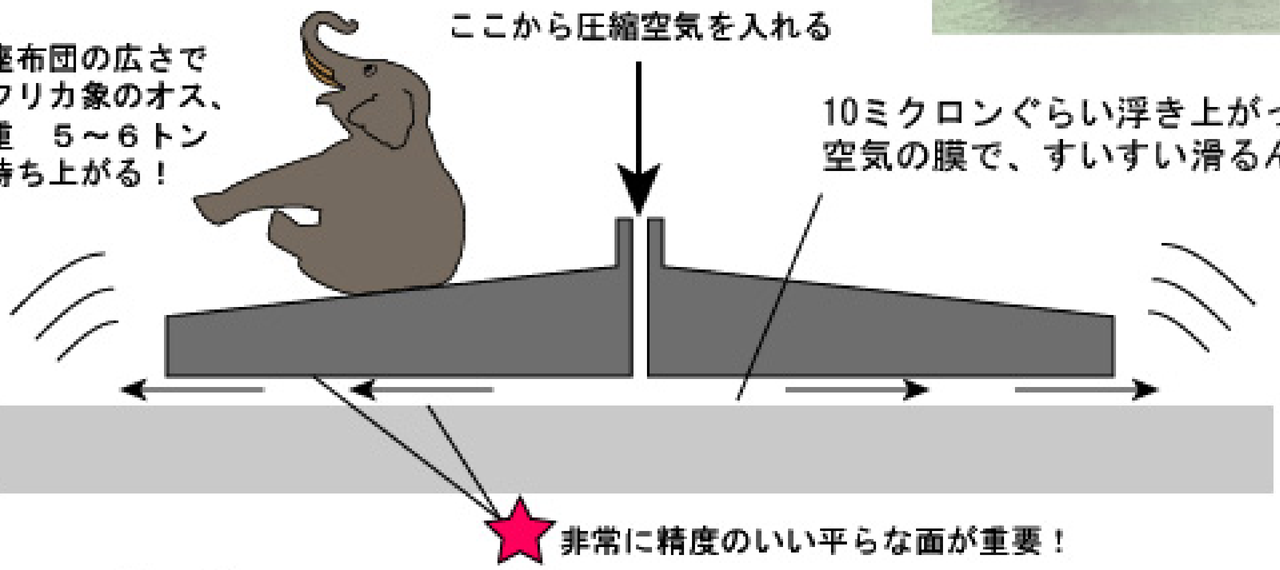

コンクリート床面研削装置



エアーパッド

空気圧は力持ち！

5 kg/cm2 x 40cm x 40 xm = 5トン



エアーパッドで
精密機械を持ち上げ
静かに移動させるんだ

6自由度を3自由度に減らして
アライメントを容易に！

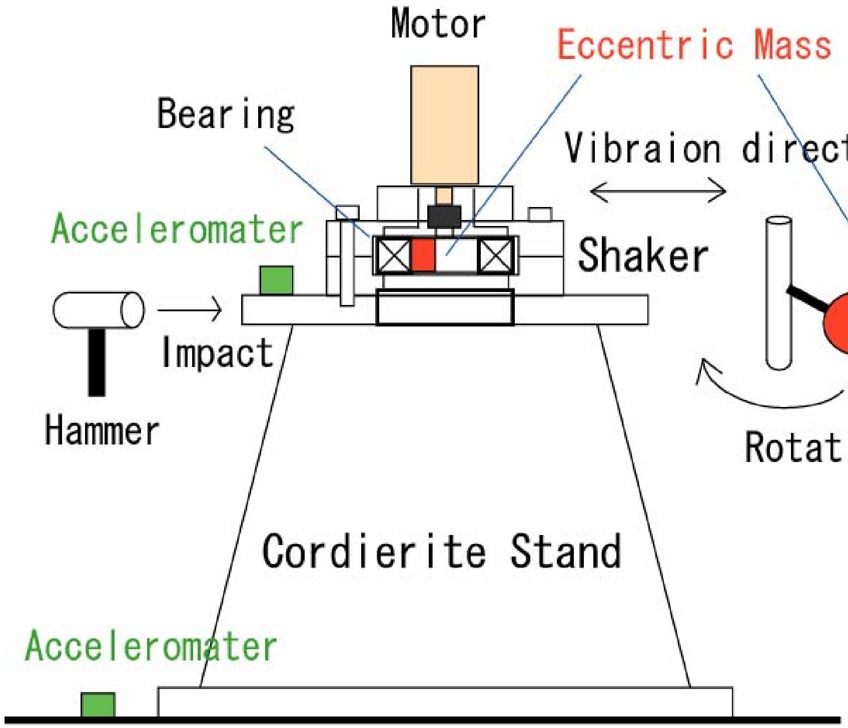
◎アライメント、位置合わせ
◎メンテナンスでの、重量物のスライド
◎フランジなど締め付け力の開放


SPring-8

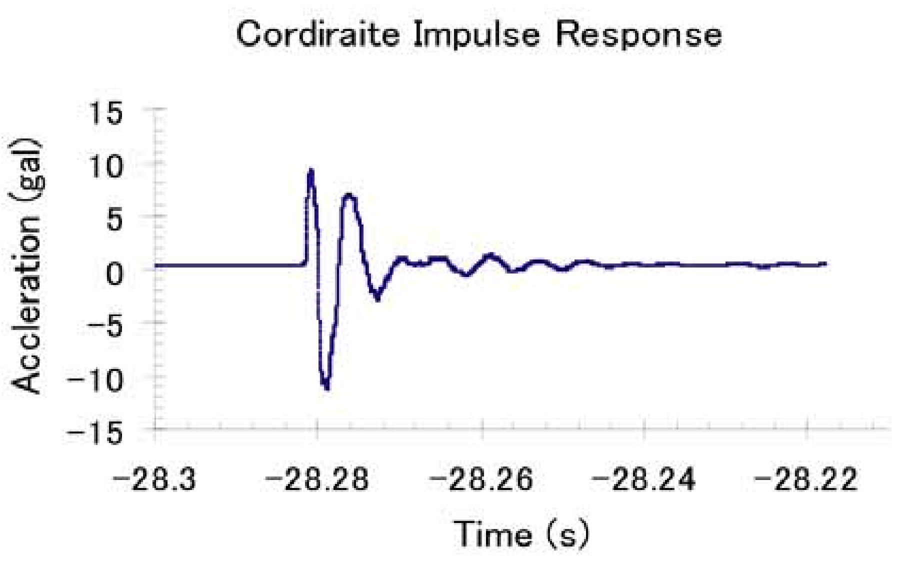

エアーパッドで
精密機械を持ち上げ
静かに移動させるんだ
これがエアーパッド
y=0
θx=θz=0
6自由度を3自由度に減らして
アライメントを容易に！
◎アライメント、位置合わせ
◎メンテナンスでの、重量物のスライド
◎フランジなど締め付け力の開放

Measurement of Vibration response of Cordierite

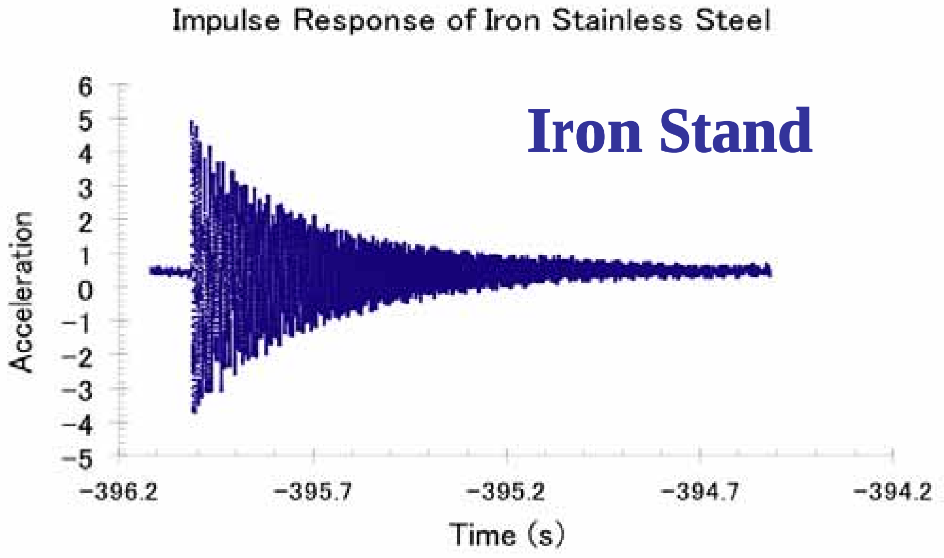
Y. Otake



Impact Response of Cordierite & Iron Stand

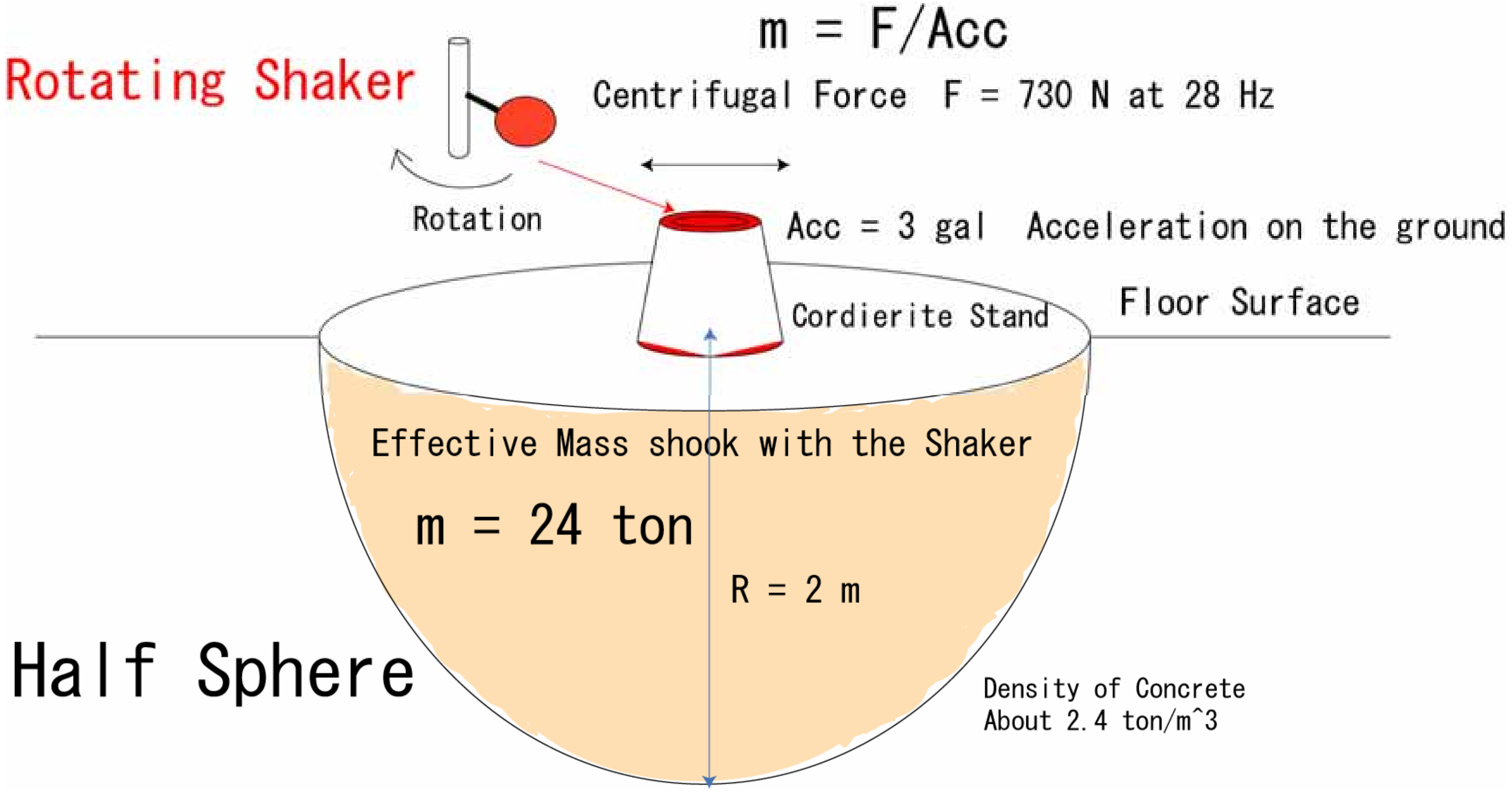


Cordierite



Iron Stand

Effective Mass shook with the Shaker



We measured the same acceleration with the accelerometers on the stand and on the floor.
This fact shows rigidity of the cordierite stand.

Radiation damage on macromolecular (protein) crystals

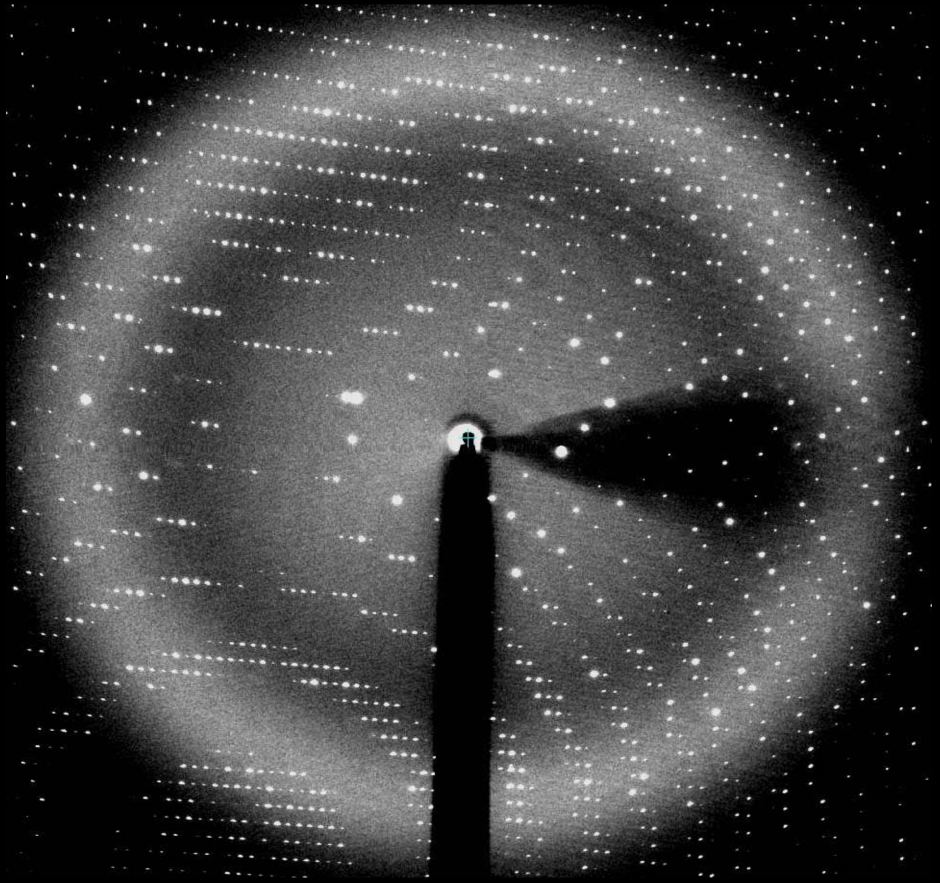
- At 10 keV X-ray, photoelectric absorption cross-section is about ten-times higher than Thomson scattering for C, N and O.

- Bragg diffraction amplifies Thomson scattering X-ray signal in crystals (through interference effect). Thus, effective photoelectric absorption effect becomes lower than Thomson scattering from 3D array of atoms in crystal.

There are big demands to analyze micro-crystals.

But!

- For smaller macromolecular crystals (< 50 micron), higher dose is required, thus radiation damage problem becomes sever.



Courtesy of M. Yamamoto

Dr. Masashi Miyano

March, 20, 2006

DRAFT

X-ray Coherent Detection and its Application to Macromolecular Crystallography

Tsumoru Shintake

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Splitting intense coherent X-ray beam from synchrotron or XFEL into two beams: low flux probe beam and high flux reference beam, followed by a sample crystal and a point reflector, respectively, overlapping two diffracted beams on a CCD detector, creating interference fringe, from which we detect the wave amplitude of diffracted beam from the sample crystal, including phase. The weak X-ray signal from the sample crystal is pumped up to higher amplitude on the reference wave due to interference effect. Most of all photons arriving on the CCD detector have bypassed the sample, thus sample damage can be lowered. Probability to detected a photon on CCD pixel is modulated by weak X-ray signal from the sample through interference effect. This method has better sensitivity for low Z-material, such as hydrogen in protein or fuel cells, which has been difficult to observe in traditional X-ray diffraction crystallography. By incorporating direct phasing method on refining phase in reference wave, we will also be able to determine the phase in diffracted wave from the sample.

1. Introduction

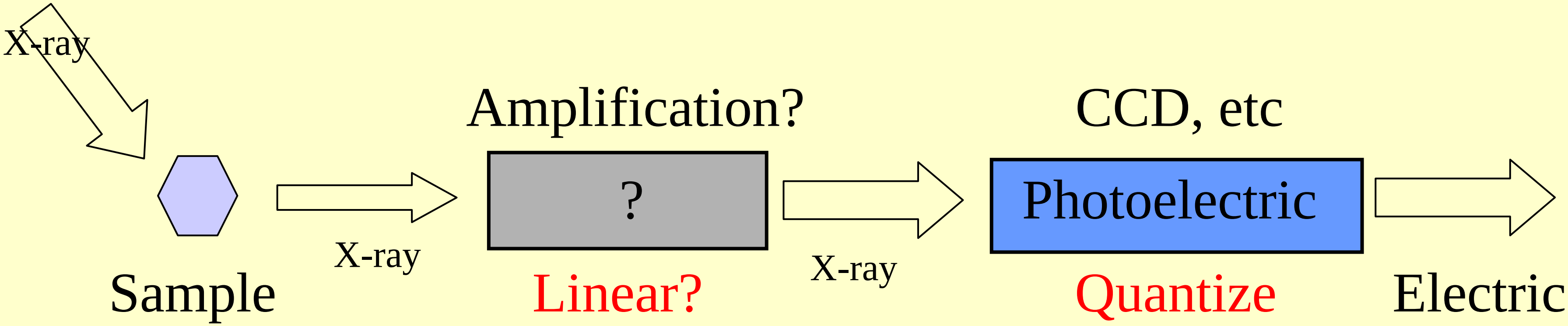
The X-ray crystallography has been established as an invaluable probe to determine three-dimensional structure with atomic resolution, in various materials, from simple compounds to more complex sample, such as DNA, and in more recent times to the structure of protein and other macromolecules in living cells. Because the structural information is a key to understand cellular processes of living cells, the X-ray crystallography is now inevitable tool in bio science, and related field.

Obtaining a suitable single crystal is the essential step in the X-ray structural analysis of protein, however, which requires many processes and sometimes years effort to grow crystals. Today's 3rd generation light source provides high intensity focused monochromatic X-ray beam, which enables to analyze smaller protein samples within reasonable exposure time. Nowadays, in the most advance beam lines, smallest sample of 100 um or below is routinely analyzed. However, there is still big demand on even smaller samples, 10 um or less, which have been wasted without analyzed in many laboratories.

How can we reduce radiation damage on macromolecular crystals

- Can we reduce X-ray flux onto sample?
- Improving the detector efficiency will reach soon the upper limit defined by single photon signal.
    - (High gain CCD, avalanche detector, or photo-multiplier)
- Once we use photoelectric effect to convert signal, we will encounter the limitation due to quantized energy as single photon.
- We have to do something before photoelectric conversion.

Can we amplify X-ray?

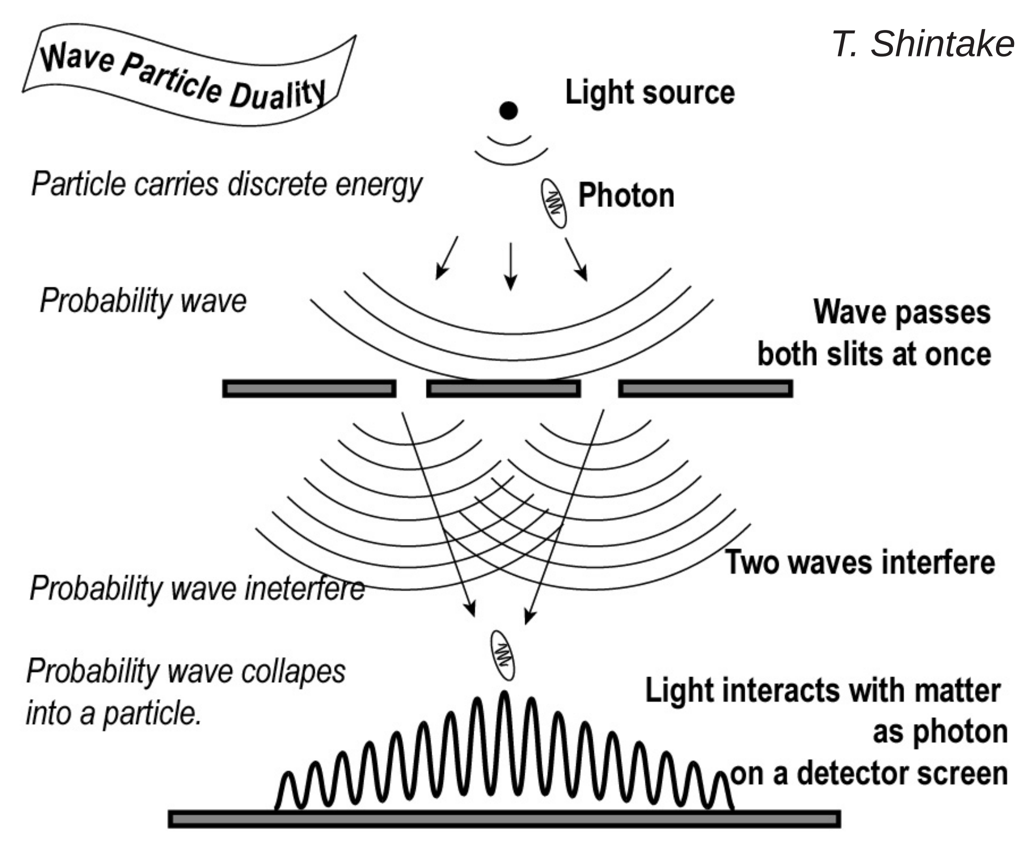


- If we use "matter" for amplification, X-ray energy will be quantize as energy of single photon, at input port.

- *X-ray laser amplifier*, needs to use matter as laser media, which also quantize the X-ray energy.

- Related to "observation theory" of particle in quantum mechanics.
- X-ray plays wave-particle duality.

Wave- particle duality of the light.



- Copenhagen interpretation of quantum mechanics formulated by Niels Bohr and Werner Heisenberg in Copenhagen around 1927.

a photon passes through two slits at the same time, as probability wave.

“Observation” needs interaction with a matter to provide signal, the probability wave collapses into a photon, and the wave energy suddenly localize at “observed location”.

Observed energy is quantized as

$$E = h\omega$$

Signal can be "pumped up" by Interference Effect between two probability waves. Amplified signal is recorded as fringe modulation on the detector.

$$I = |\psi|^2 = \psi^* \psi = \left(\psi_1{}^* + \psi_2{}^*\right)\cdot\left(\psi_1 + \psi_2\right)$$

$$= |A_1|^2 + |A_1||A_2| \exp i(\phi_1 - \phi_2) + |A_1||A_2| \exp i(-\phi_1 + \phi_2) + |A_2|^2$$

$$= |A_1|^2 + 2|A_1||A_2| \cos(\phi_1 - \phi_2) + |A_2|^2$$

$$\approx |A_2|^2 \left\{1 + 2\frac{|A_1|}{|A_2|}\cos(\phi_1 - \phi_2)\right\}$$

$$= I_2 \left\{1 + 2\sqrt{\frac{I_1}{I_2}}\cos(\phi_1 - \phi_2)\right\}$$

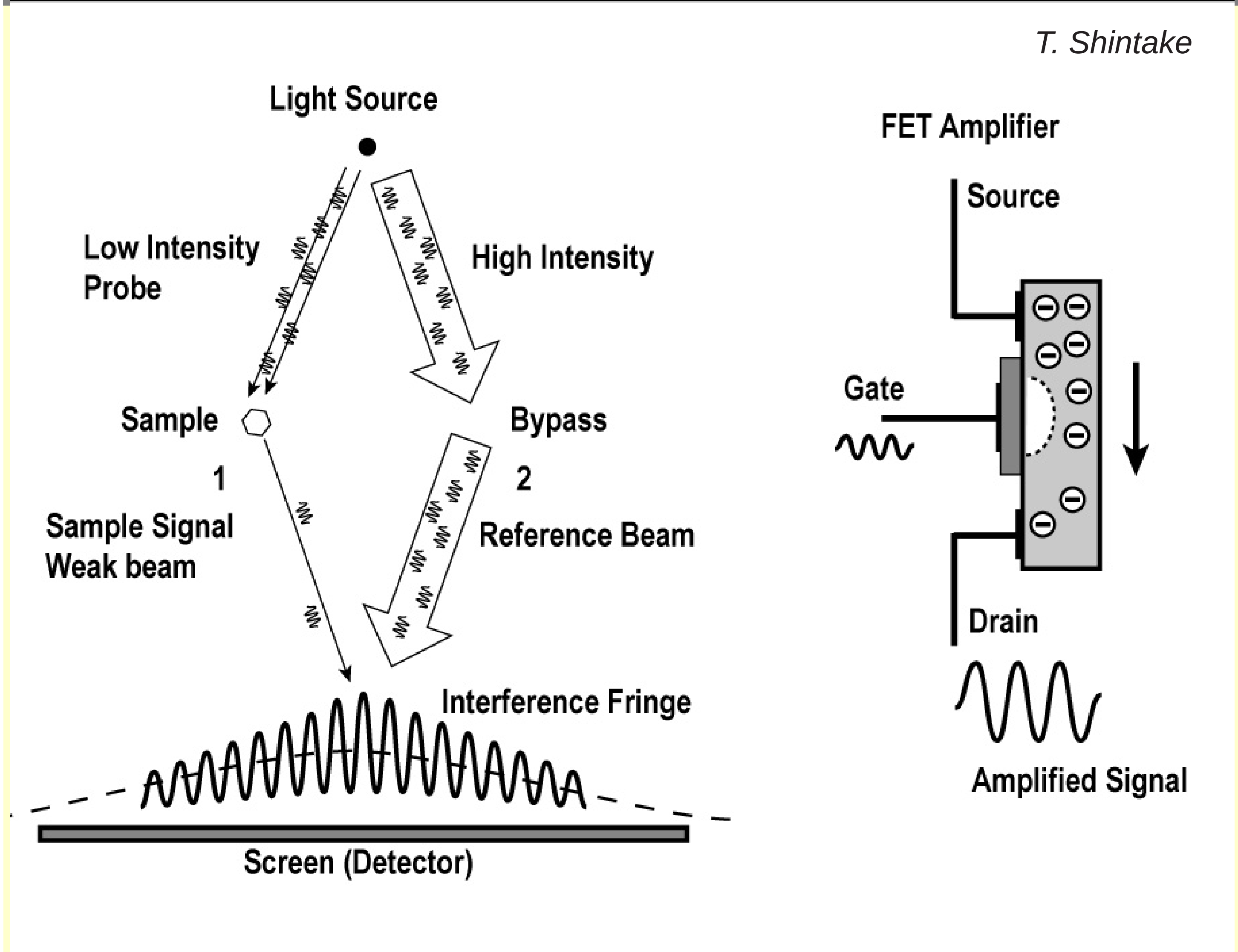
$$\Delta I = 4 I_2 \sqrt{\frac{I_1}{I_2}}$$

$$I_1 = 0.01,\ I_2 = 1 \quad \rightarrow \Delta I = 0.4$$

$$I_1 = 0.0001,\ I_2 = 1 \quad \rightarrow \Delta I = 0.04$$

I_1 signal is amplified 40 times,
400 times gain.

Bypass main beam, and detect sample with low intensity probe beam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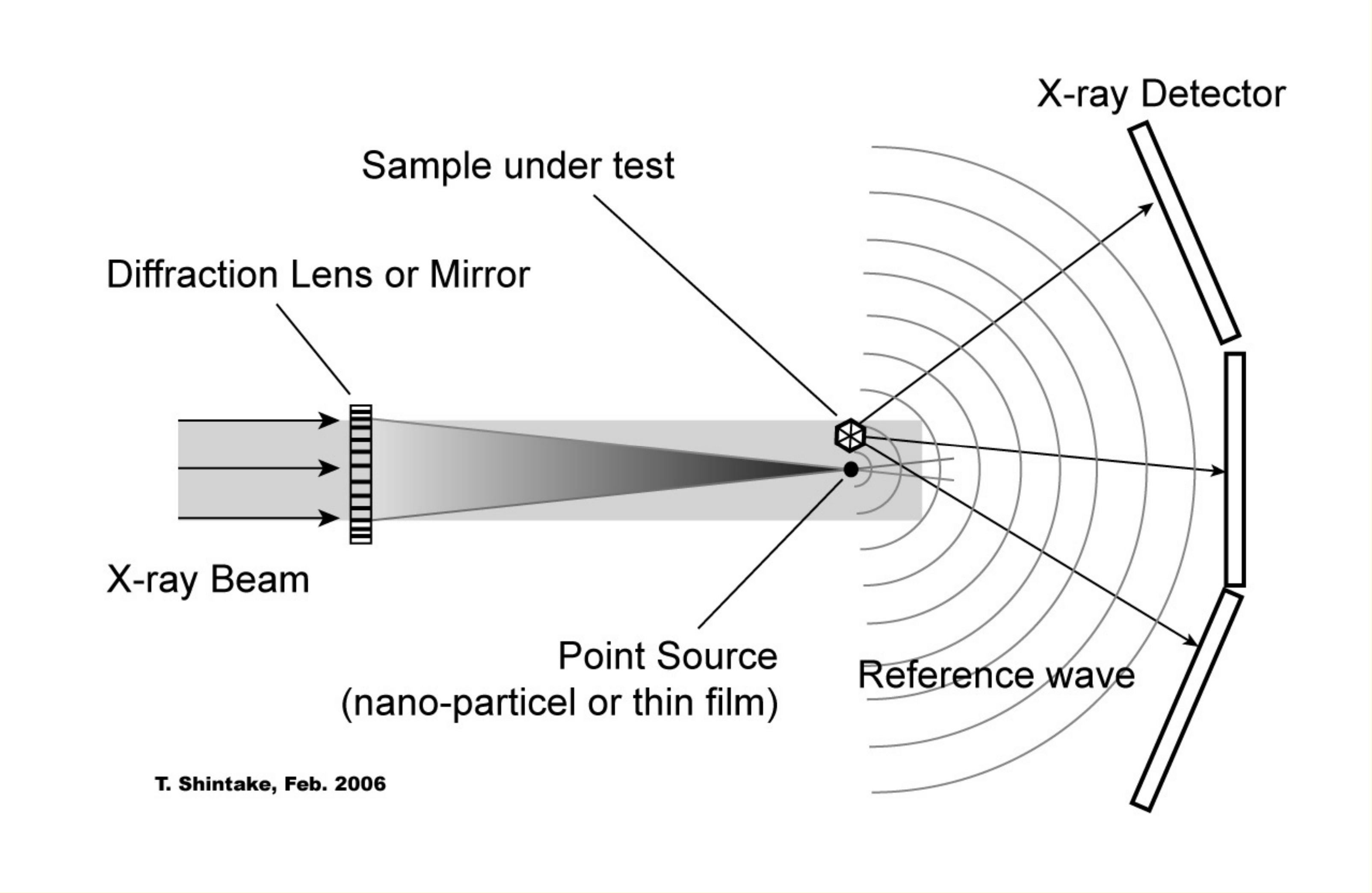
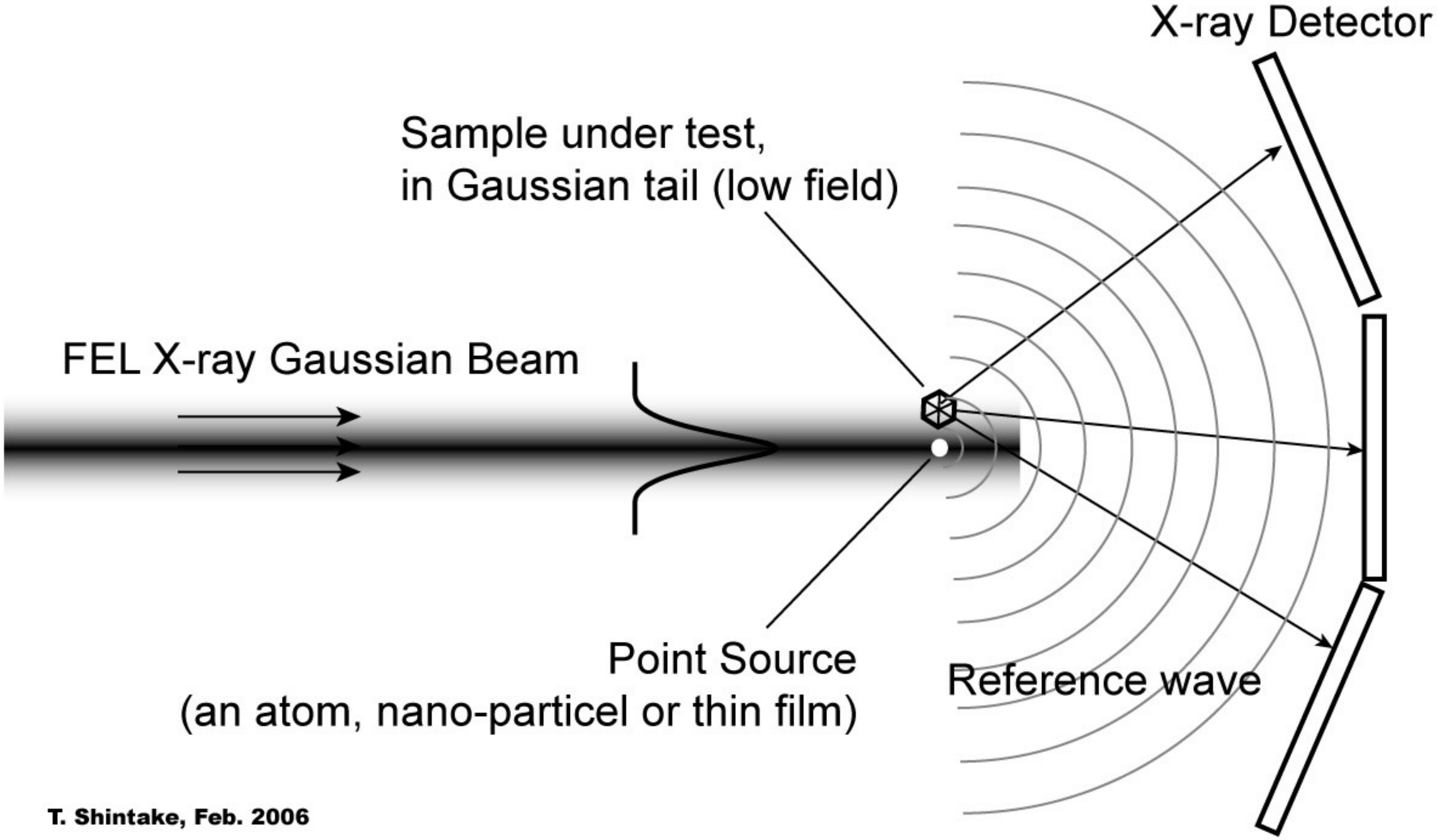
Weak sample signal from Arm-1 modifies (controls) distribution of high intensity beam of Arm-2 at the screen.

Analogy is FET transistor, gate signal controls flow of carrier.

How to realize in crystallography? Gabor Holography Configuration with much higher reference wave for pumping.



XFEL case.


X-ray Detector
Sample under test,
in Gaussian tail (low field)
FEL X-ray Gaussian Beam
Point Source
(an atom, nano-particel or thin film)
Reference wave
T. Shintake, Feb. 2006

Required Conditions

- Fringe pitch ~ 100 micron-meter.
- Distance between point-reflect to sample, and detector.
  - L = 1 m.
  - D = 1 micron-m
  - Wavelength = 1 Angstrom
- Detector Resolution < 30 micron-meter.
- X-ray Coherent Length > point-reflector to sample distance. ~ 3 micron-meter.(3 x 10^4 Angstrom)
- Detector Area Size
  - Resolution of crystal analysis ~ 1 Angstrom
  - θ = 30 degree.
  - Detector Area 1 m x 1 m
  - 33 k x 33 k = 1 G pixel.
- Gain, or damage reduction.
  - 12 bit ADC on CCD, 2048 level at middle as reference wave, lets a few bit as minimum detectable modulation, 10^{-6} signal from sample will be amplified to 10^{-3} , thus gain is x 1000.

$$p = \frac{\lambda}{\theta} = \frac{\lambda L}{D}$$

$$|S| = \frac{2\sin\theta}{\lambda}$$

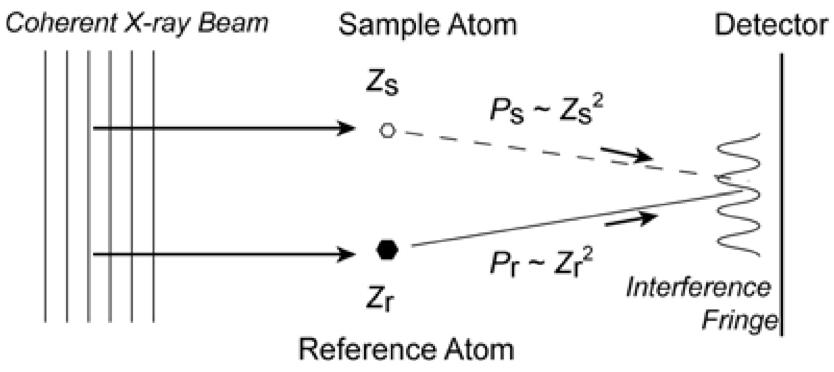


Fig. 2 Two atoms diffraction and interference.

The trick of this gain is due to the fact that the wave interferes is described by mathematical linear sum of amplitudes, but its probability density or power is given by its square.

If we define power gain as ratio of modulation term in eq. (2.4) to the signal power P2, we find

$$G = \frac{4\sqrt{P_1 P_2}}{P_2} = 4\sqrt{P_1 / P_2} \qquad (2.5)$$

If we can apply this scheme to X-ray crystallography, especially protein crystallography, we may detect low mass atoms. The power of the diffracted X-ray from an atom, which is known as the atomic form factor, is approximately proportional to Z^2.

$$P_Z \propto Z^2 \qquad (2.5)$$

Therefore the diffracted X-ray from low atomic number becomes drastically small, and hard to detect the hydrogen atoms in protein. However, it is believed that the hydrogen itself plays most important function in biological activities, and desire to see hydrogen atom is always exits.

If we utilize interference effect, from eq.(2.4), the Z-dependency becomes

$$P_Z \propto Z$$

Therefore, power dependency on atomic number becomes linear and the detection of low Z-material becomes easier.

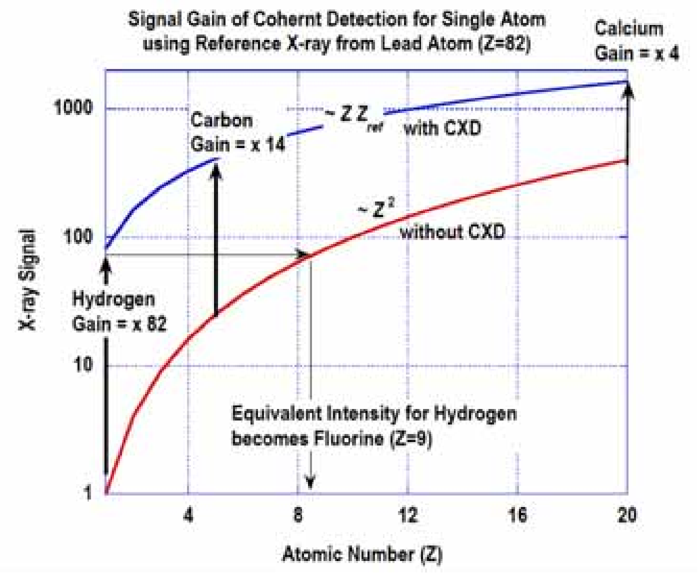


Fig. 3 Effective form factor.

The Point Reflector

- Point reflector has to scatter X-ray homogeneously in 2 π space. (no interior structure is desirable)
- It will be
  - amorphous micro-ball
  - or thin film
  - of heavy material,
  - or amorphous ice around protein crystal.

- Or single atom, in case of XFEL.

Challenge for Phase Determination

- Amorphous point reflector provide back ground illumination, which becomes speckle.
- Speckle phase can be determined by blocking sample radiation, and apply phase retrieval using over sampling, where the small angle diffraction will provide boundary condition of initial phase near the axis. $\rightarrow \phi_2$
- Wave number of phase variation of speckle is much slower than Bragg diffraction spot from crystal, we can interpolate phase of reference wave in the Bragg spot.
- From the fringe phase, we determine phase difference, thus determine phase of crystal diffraction.

$$\cos(\phi_1 - \phi_2) \rightarrow \quad \phi_1 - \phi_2 \quad \rightarrow \quad +\phi_2 \quad \rightarrow \phi_1$$

- **Effect of Mosaic block has to be studied carefully.**

To Improve Coherency in XFEL

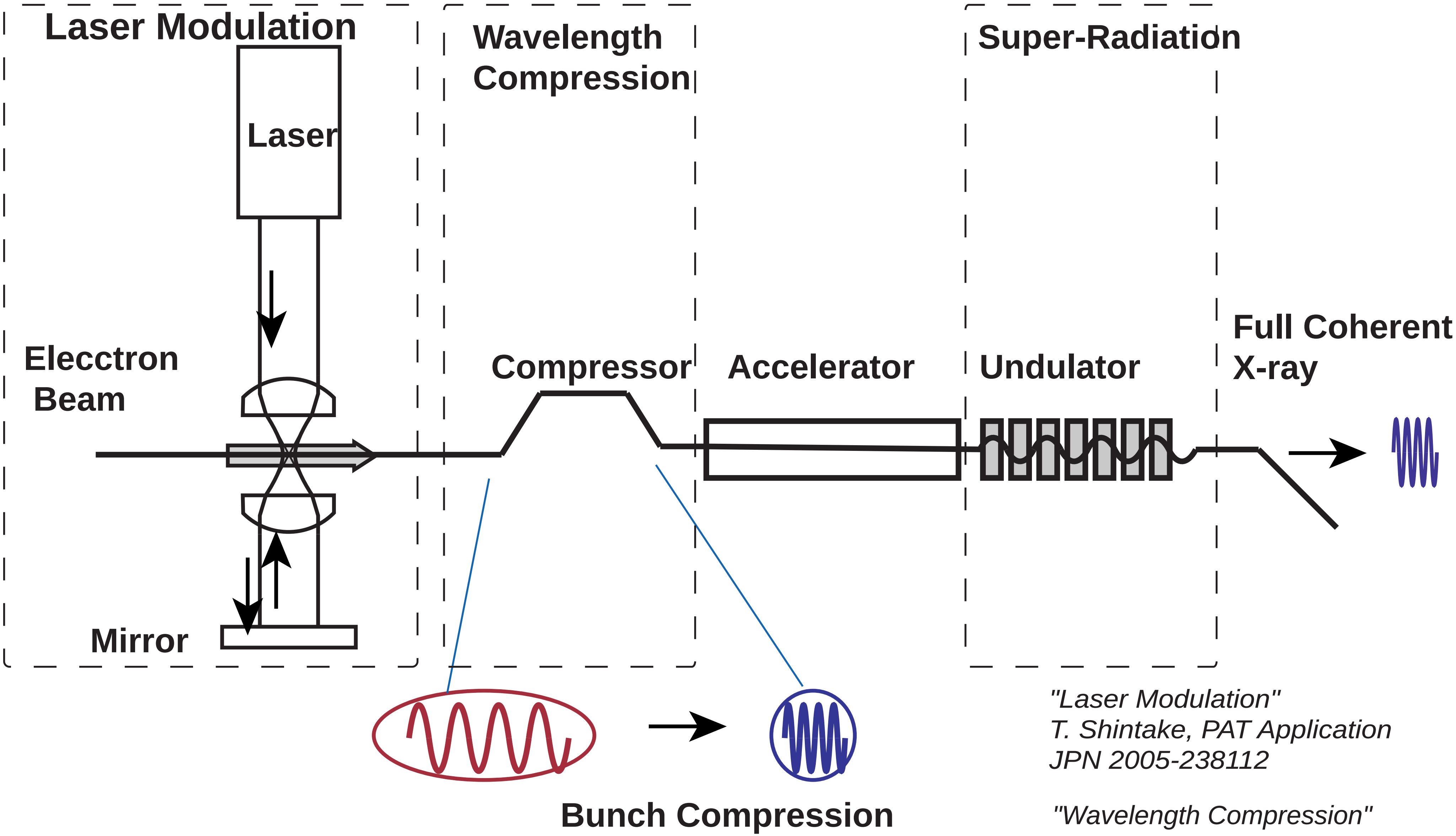
- SASE-FEL light is not fully longitudinally coherent = there are many longitudinal modes.
  - This is due to SASE-FEL starts from spontaneous (noise) undulator radiation.
  - Using coherency is limited.

- HGHS with optical seeding will provide fully coherent light, but limited 1 nm or longer wavelength.

- Laser Modulation + Wavelength Compression will provide a possible path to realize fully coherent X-ray at 1 Angstrom region.
  - Full coherent
  - Variable power from zero to maximum
  - Atto-second pulse generation is possible
  - A few undulators are enough.
  - Tolerate electron parameter (lower current, moderate emittance)
  - CSR effect help to transfer modulation.
  - Need careful study on smearing effects.

Laser Modulation and Wavelength Compression

T. Shintake
2005.08



Laser Modulation

Wavelength Compression

Super-Radiation

Laser

Elecctron Beam

Compressor

Accelerator

Undulator

Full Coherent X-ray

Mirror

Bunch Compression

"Laser Modulation"
T. Shintake, PAT Application
JPN 2005-238112

"Wavelength Compression"
T. Shintake, 1999
KEK AccLab-99-1

Conclusion

- Coherent X-ray detection scheme will contribute to reduce radiation damage on macro-molecular crystals.

- It also possible to provide phase information of diffracted X-ray from crystal.

- Hydrogen can be detected.

- Need effort to make high resolution, wide area X-ray detector.
- Need to improve FEL coherent length. >10 micron
  - Seeding
  - Laser-modulation + wavelength compression
  - Monochrometer in SASE.