High Energy Accelerator Research Organization (KEK)
Institute of Materials Structure Science (IMSS)
PF Photon Factory

XDL2011
RPCC, Cornell Univ.
June 20-21, 2011

Toward Fourier-limited X-ray Science

Photon Factory, KEK
& PREST, JST

Shin-ichi Adachi

outline

- Time-domain X-ray science
  - with Storage Ring (Photon Factory Advanced ring, KEK)
- Current status of Energy Recovery Linac (ERL) project at KEK
  - 35-245MeV ERL test facility (under construction)
  - 3.5GeV ERL + XFEL Oscillator (not approved)
- Towards Fourier-limited X-ray Science with XFEL-O and seeded XFEL
  - Inelastic X-ray scattering
  - Nonlinear X-ray Optics
  - Two-photon correlation spectroscopy
  - Transient grating
- Summary

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TR x-ray applications at KEK

Picosecond photoresponse of perovskite manganite (NSMO) thin film (τ~ 50ps ~ 2ns)

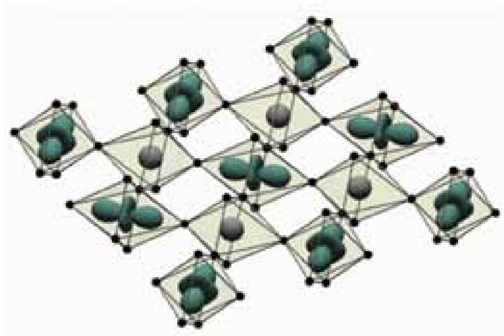
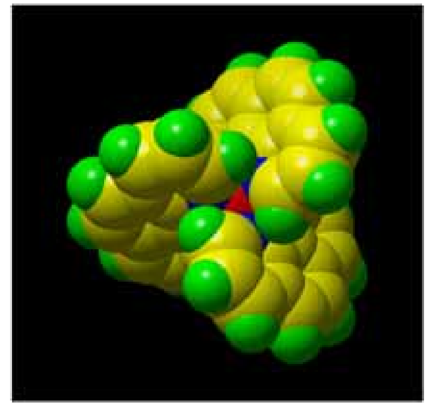
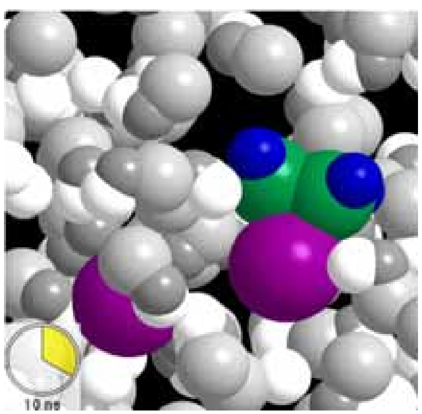


Photo-induced spin-crossover transition of metal complex in solution

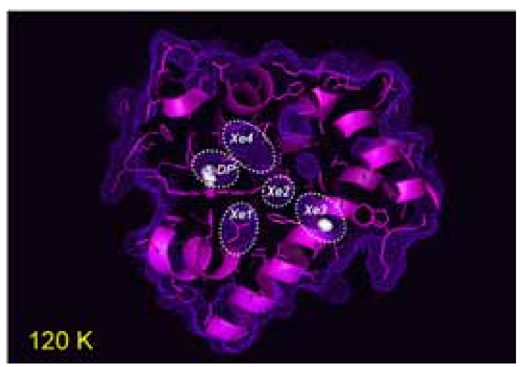
(TR-XAFS: τ ~700ps)



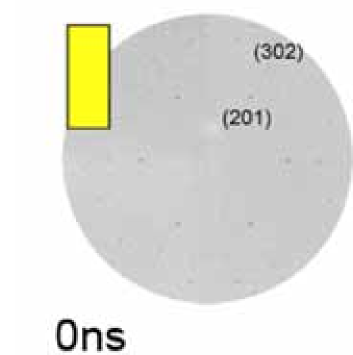
Photochemical reaction in liquid (TR-liquidography: τ~100ps~1μs)



Ligand migration dynamics in protein crystal (τ~800 min)



Laser shock-induced lattice deformation of CdS single crystal (TR single-shot Laue diffraction: τ~1ns~10ns)



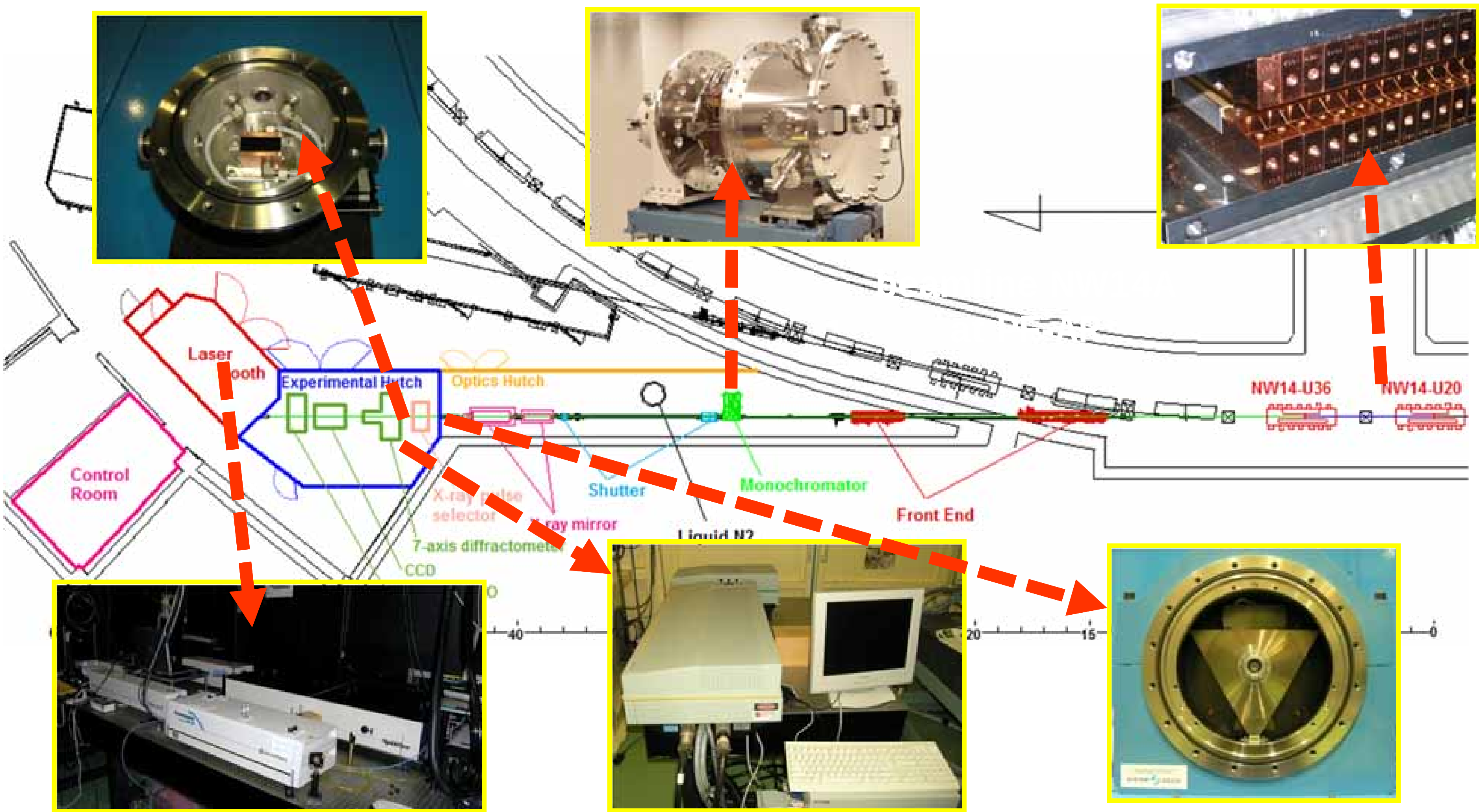
PF-AR (6.5GeV) Full-Time Single-Bunch Operation

~200days/year

multilayer mirror

Si(111) monochromator

undulator



femtosecond laser system

nanosecond laser system

Jülich x-ray chopper

#1 TR-Diffraction

Picosecond photoresponse of perovskite manganite (NSMO) thin film

1 kHz rep rate

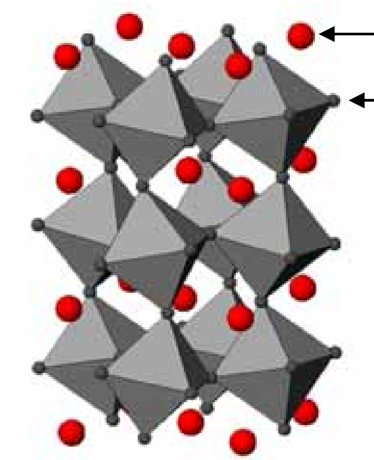
with mono X-ray ($\Delta E/E$ ~ 0.01%)

~10^9 photons/sec

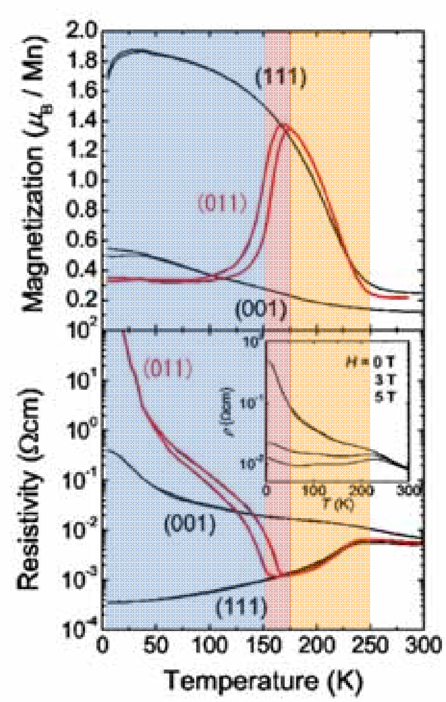
Phase Transition in Manganite Thin Film

Ichikawa *et al.*
Nature Materials,
10, 101-105 (2011)

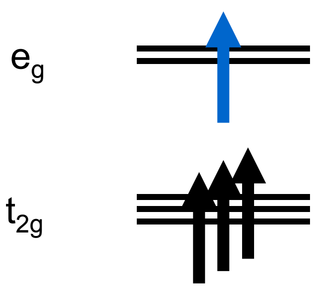
$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$
(NSMO/STO(011))

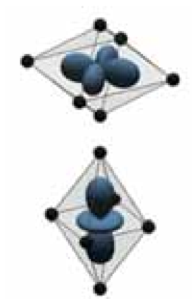


thickness: 80 nm



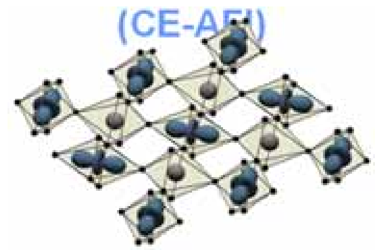
Mn^{3+}: $(3d)^4$



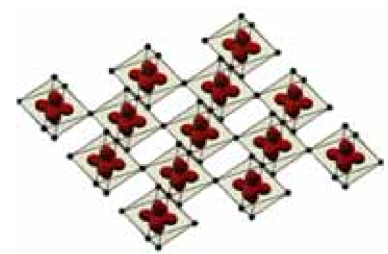


Nakamura *et al*. APL **86** 182504 (2005)

CE-type Antiferromagnetic insulator (CE-AFI)

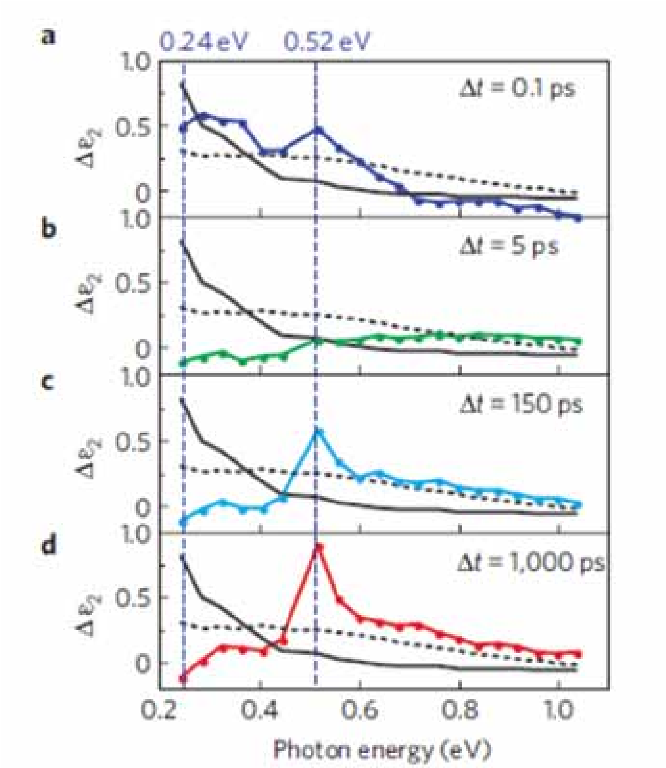


Ferrometal (FM)



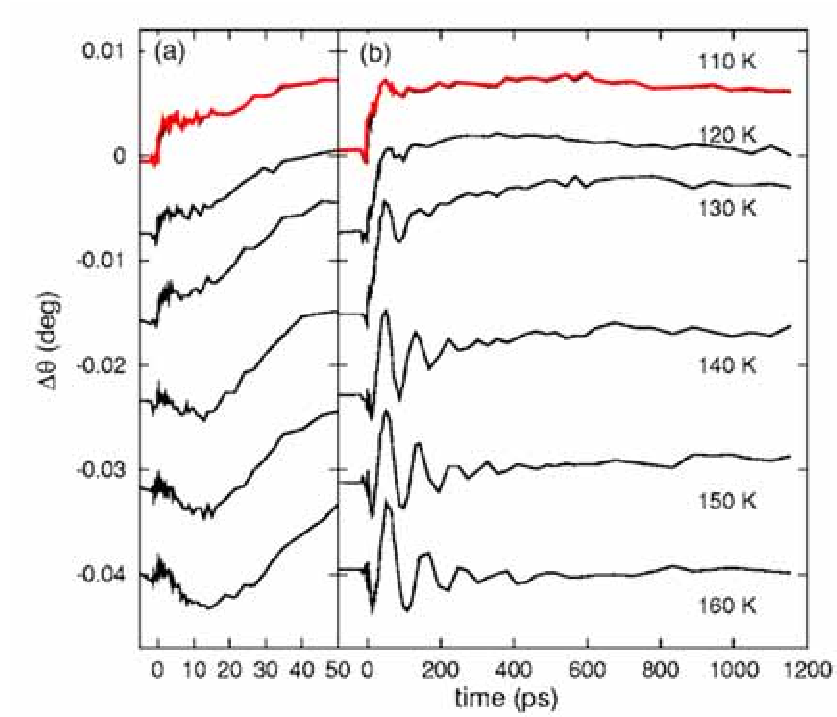
Optical pump-probe results
Collaboration with K. Miyano Group (Univ. of Tokyo)

TR-Reflectivity (100K)



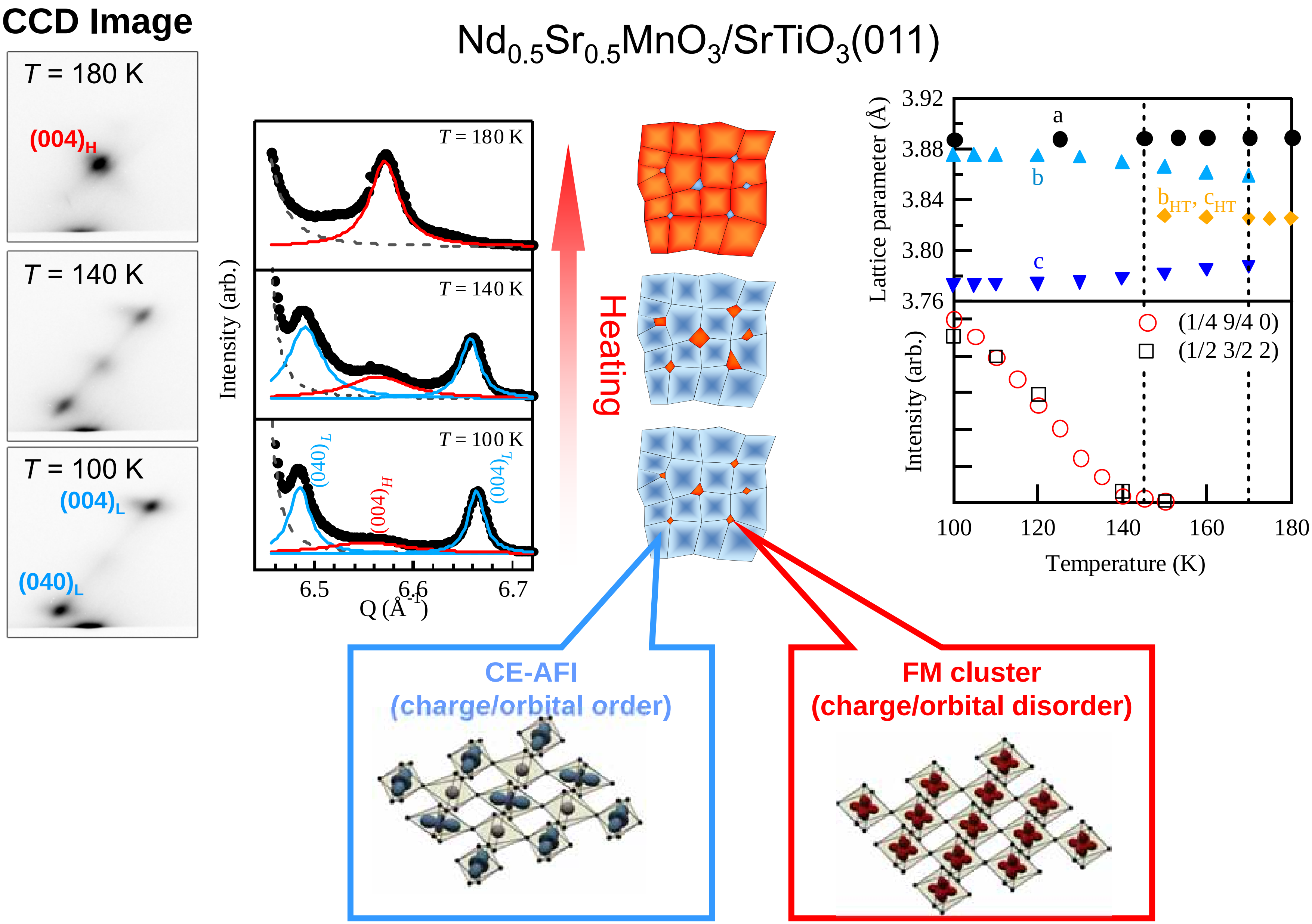
Ichikawa *et al.*
Nature Materials, 10, 101-105 (2011)

Kerr Rotation

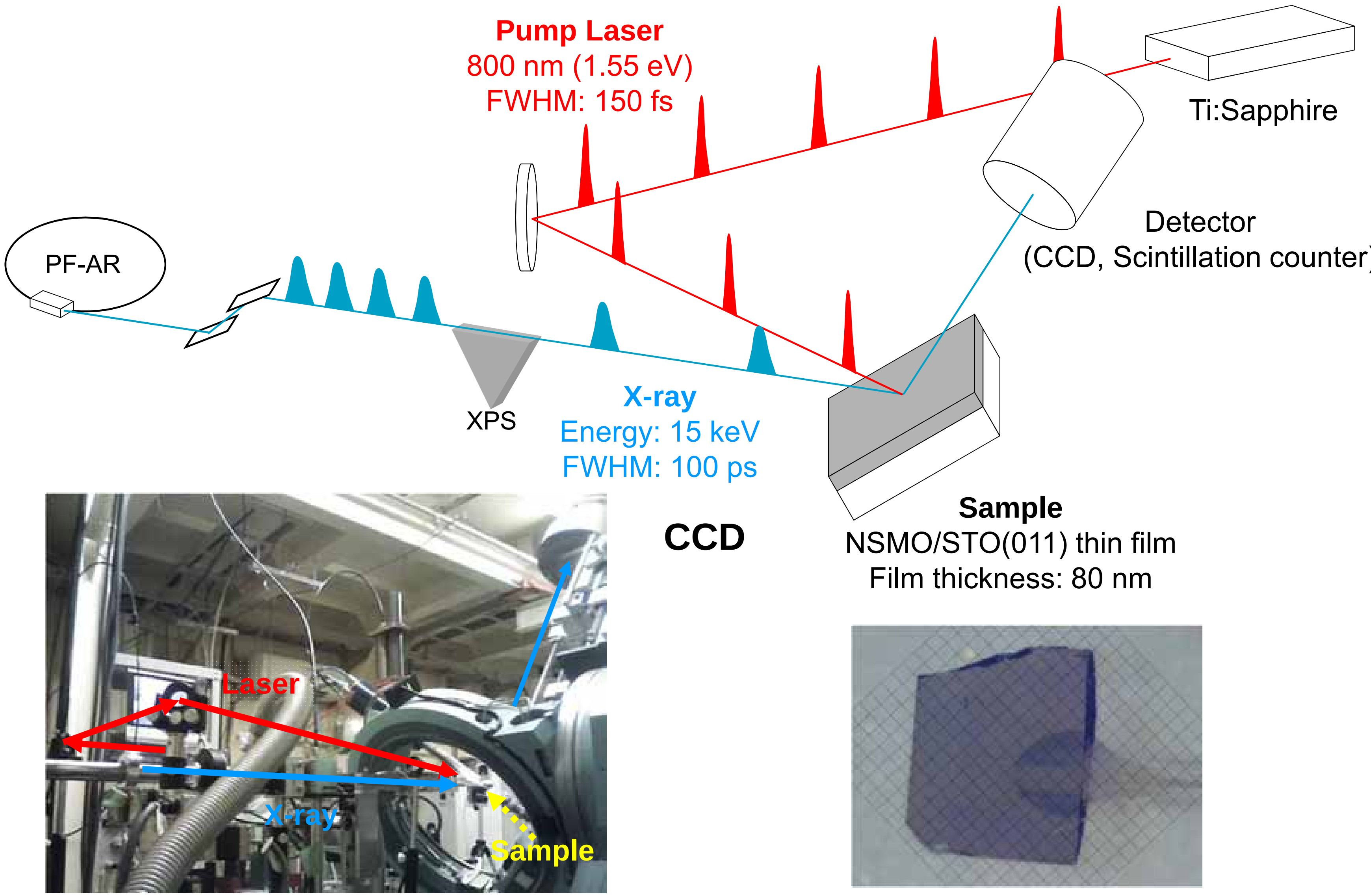


Miyasaka *et al*. PRB **74** 012401 (2006)

Temperature dependence of X-ray Diffraction



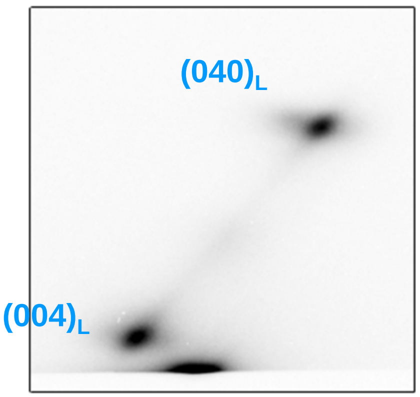
Layout of the laser-pump X-ray-probe experiment



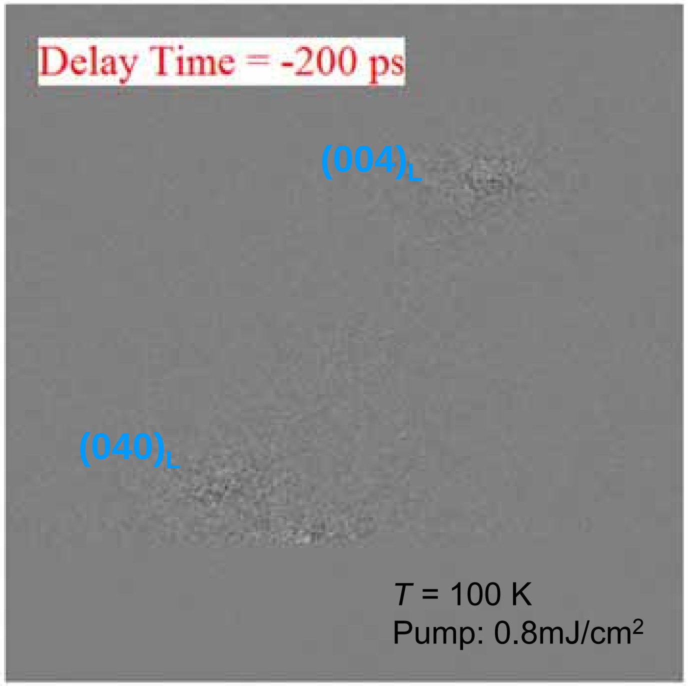
Time dependence of (004) reflection

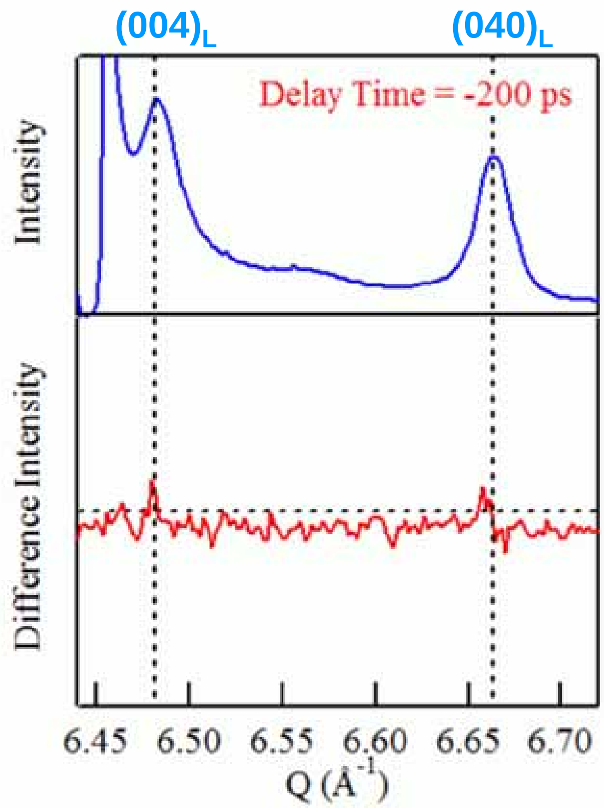
$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$

T = 100 K



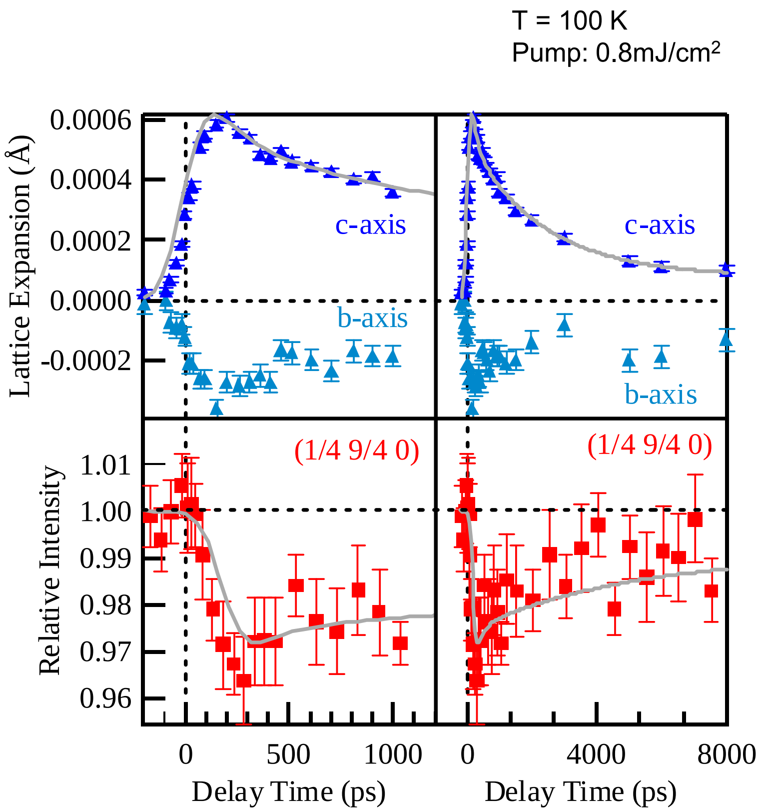
Difference Image
black：+ white：−





Time dependence of the (004) and (1/4 9/4 0) reflections

$Nd_{0.5}Sr_{0.5}MnO_3/SrTiO_3(011)$



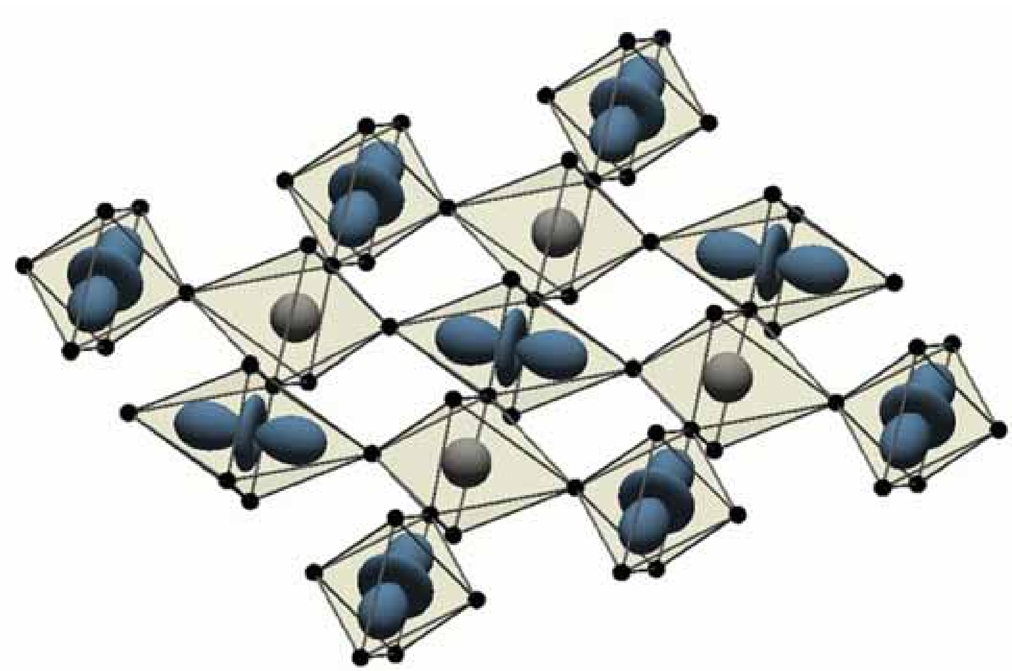


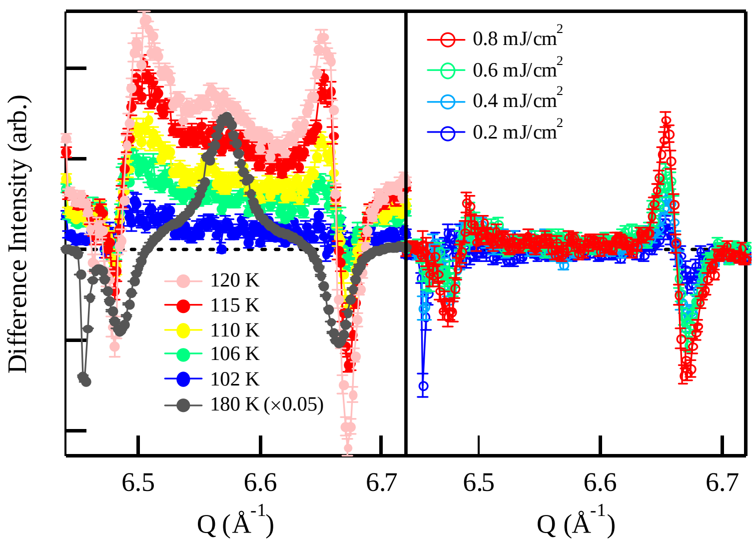
Photo-induced “hidden” state?

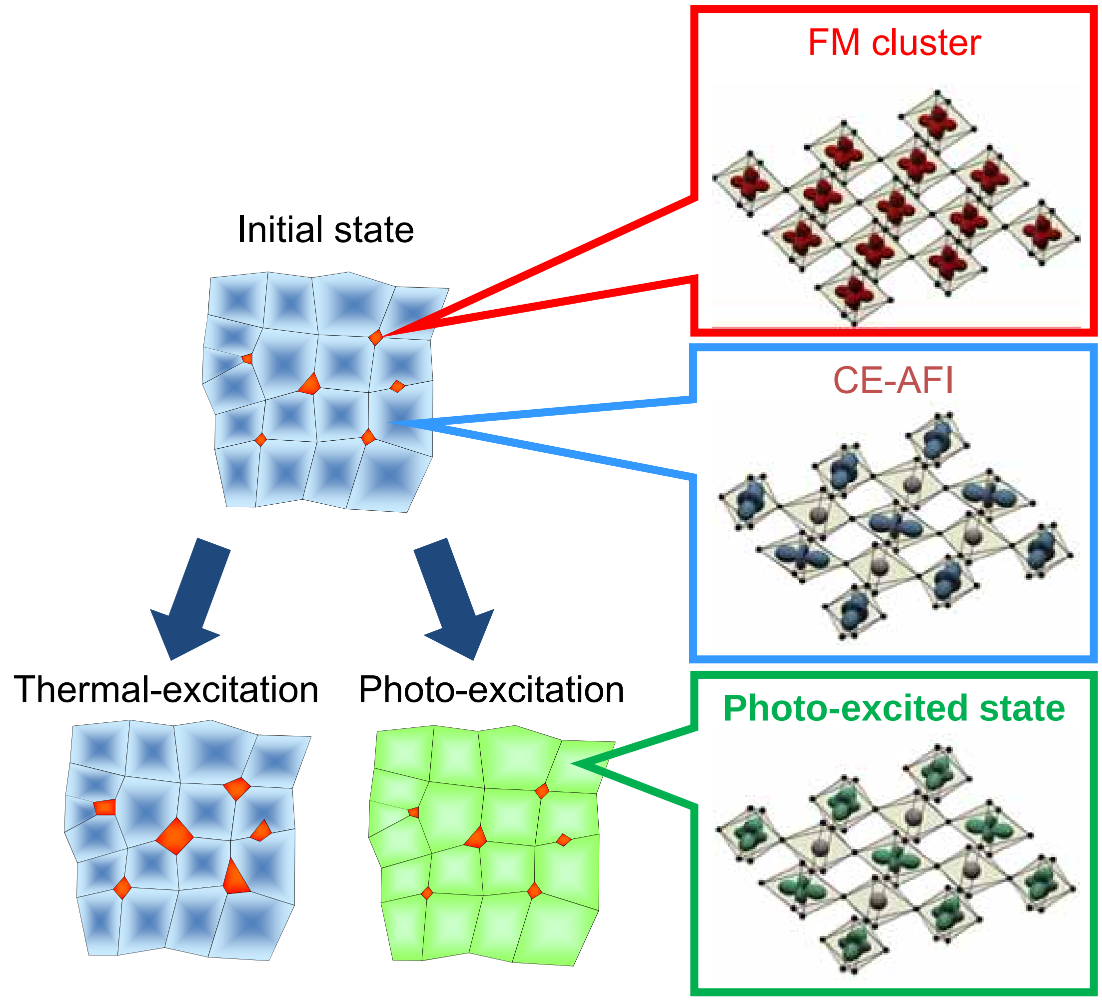
Temperature Dependence

(Without laser irradiation)

Pump Power Dependence

T = 100 K
(Delay-time: +150 ps)





Ichikawa et al.
“Transient photoinduced ‘hidden’ phase in a manganite”
Nature Materials, 10, 101–105 (2011)

#2. TR-XAFS

Photo-induced spin-crossover transition of metal complex in solution

1 kHz rep rate

with mono X-ray ($\Delta E/E$ ~ 0.01%)

10^9 photons/sec

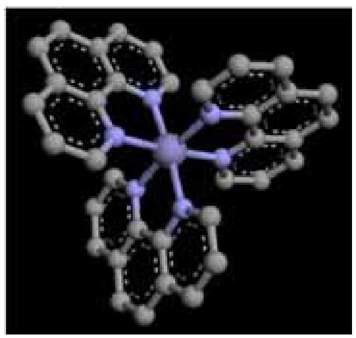
Nozawa *et al.* **J. Am. Chem. Soc., 132**, 61-63 (2010).

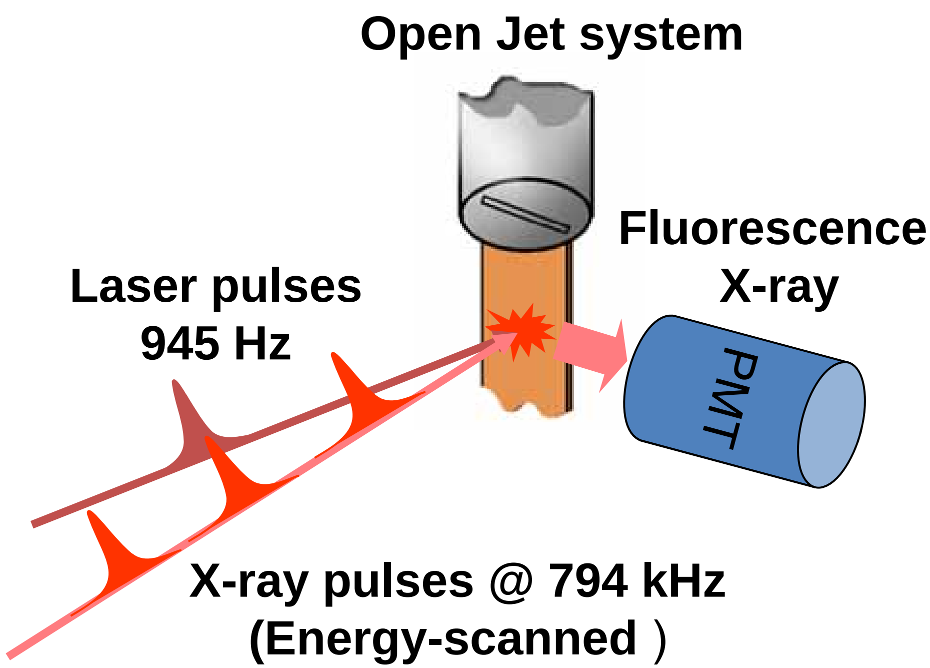
photo-induced spin-state transition by TR-XAFS

Shunsuke Nozawa (KEK)

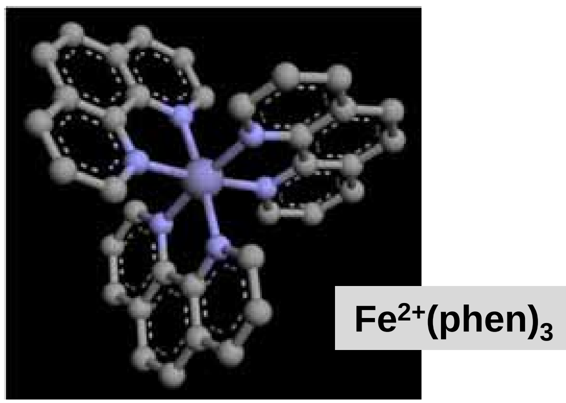
Tokushi Sato (KEK)

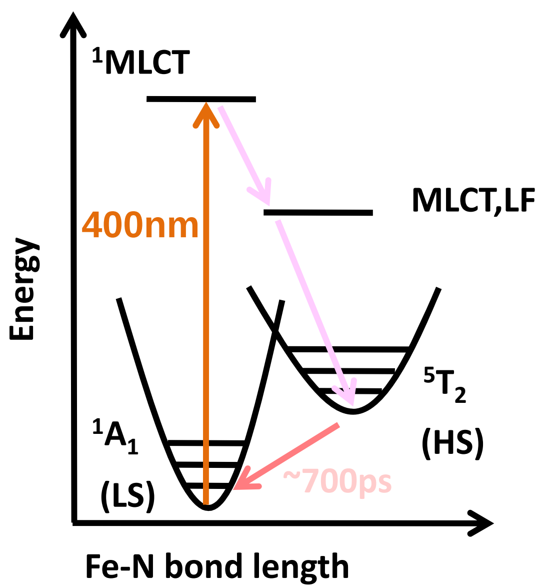
$Fe^{2+}(phen)_3$

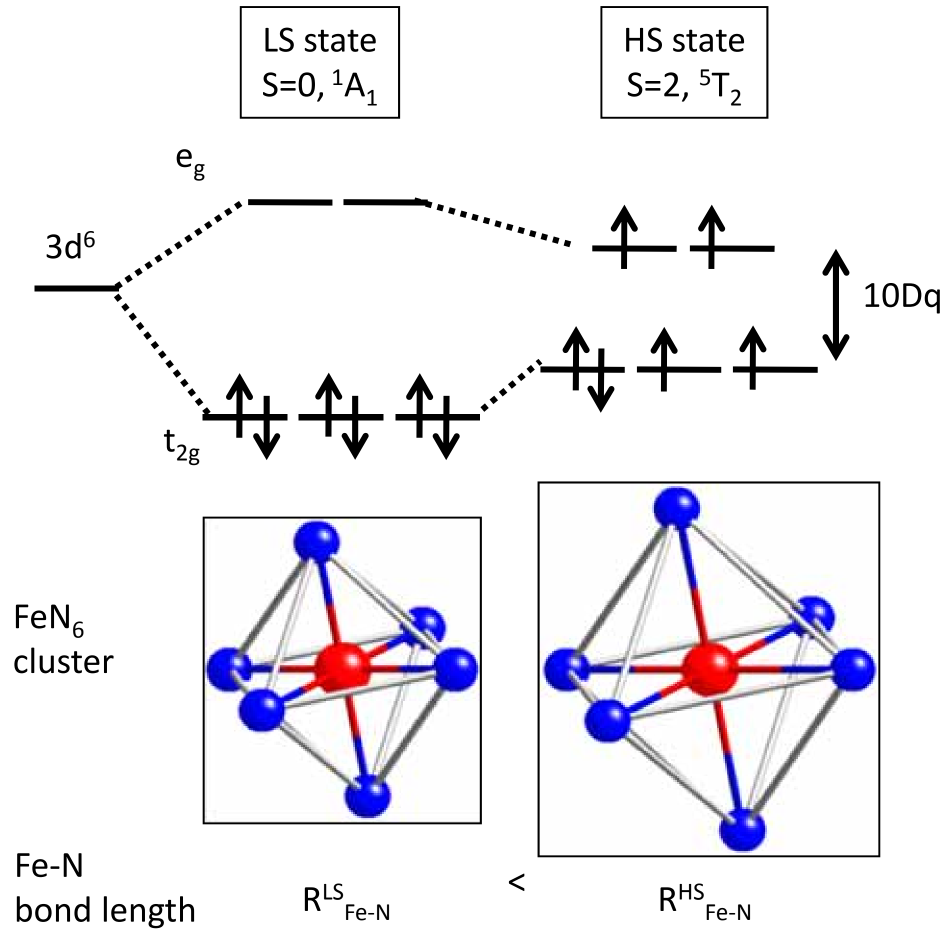




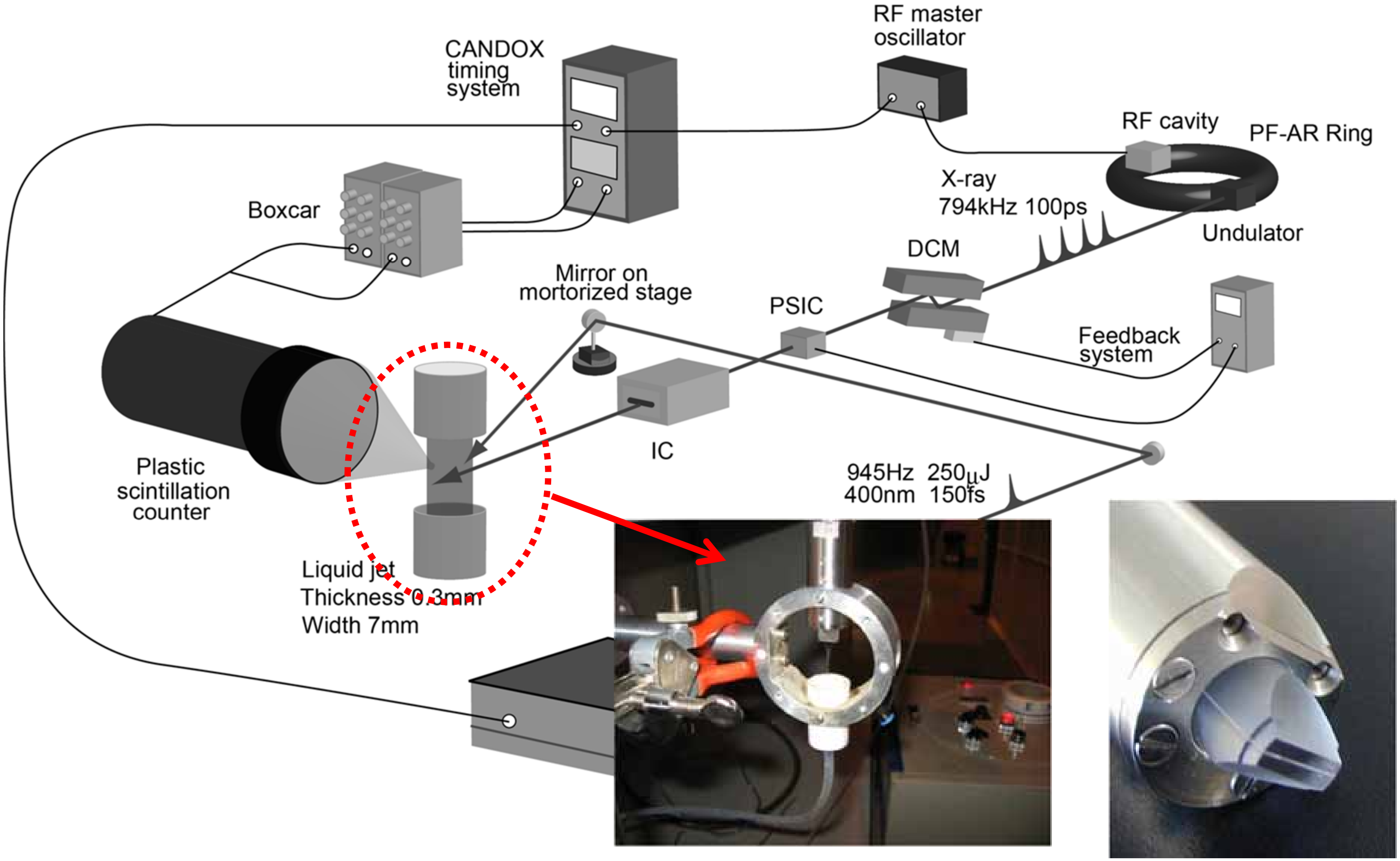
picosecond time-resolved spin-crossover transition of $Fe^{II}(phen)_3$



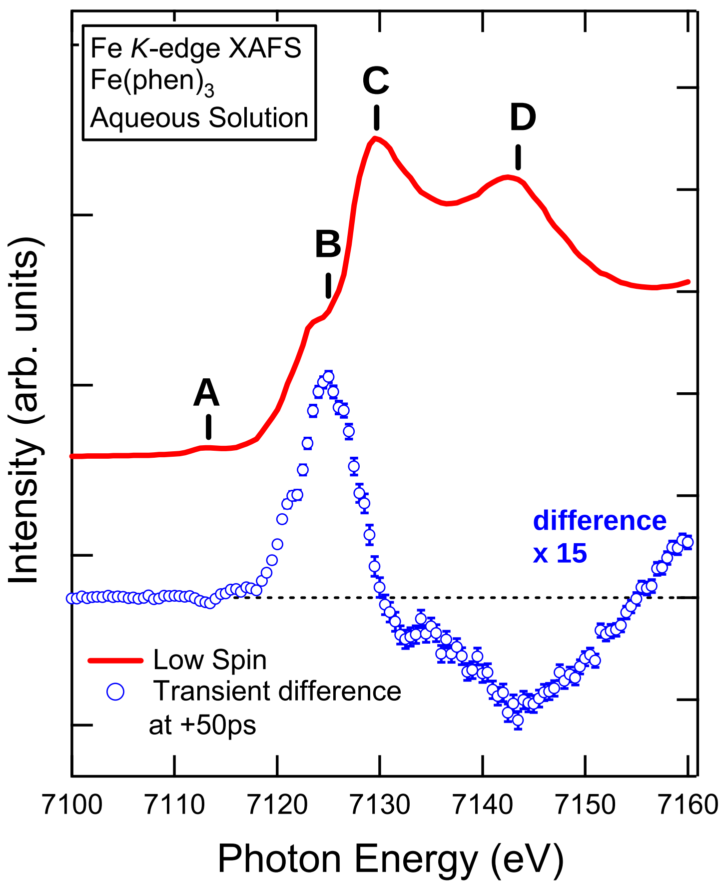


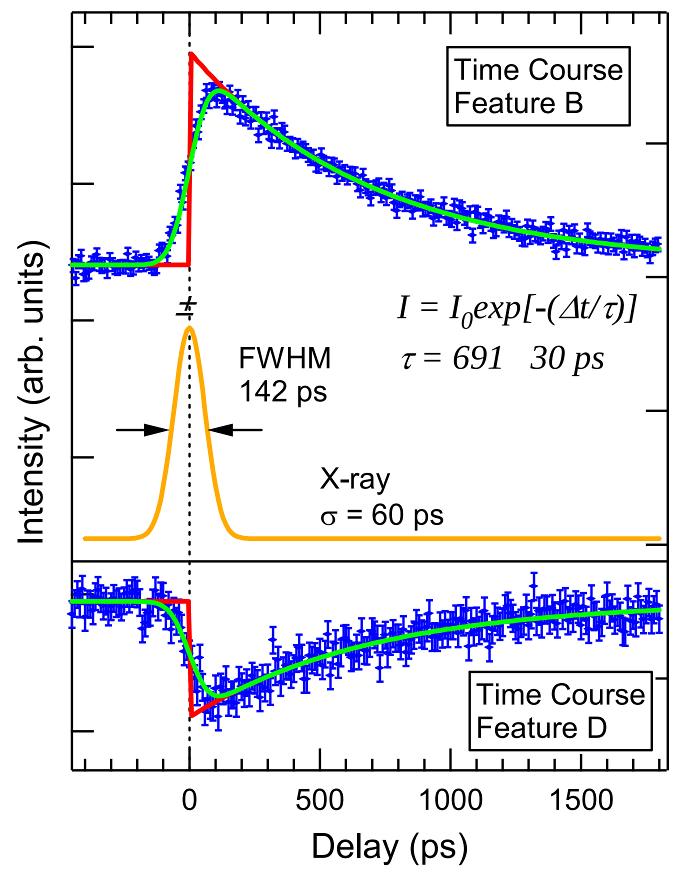


TR-XAFS: Experimental Setup

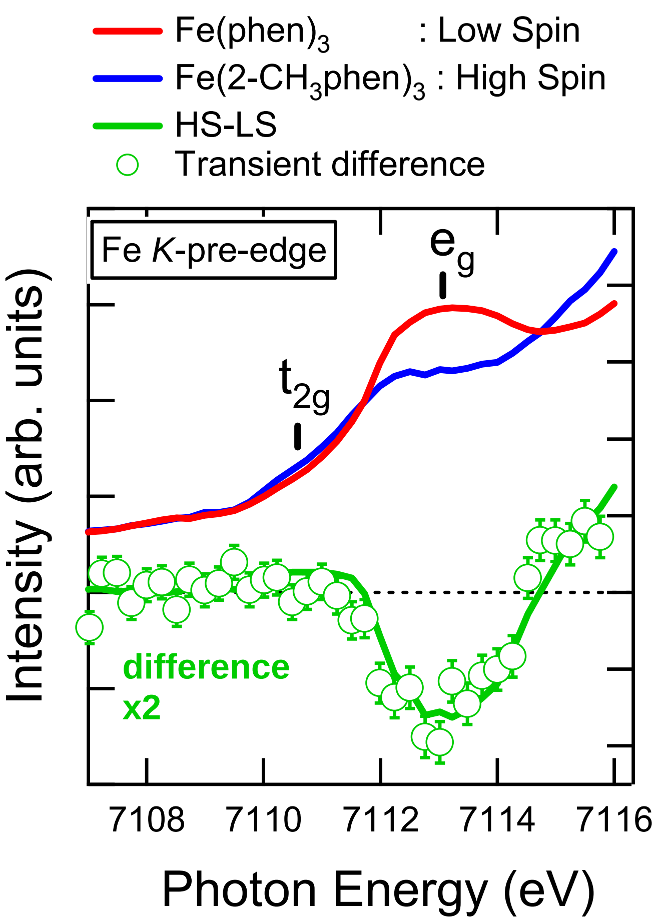


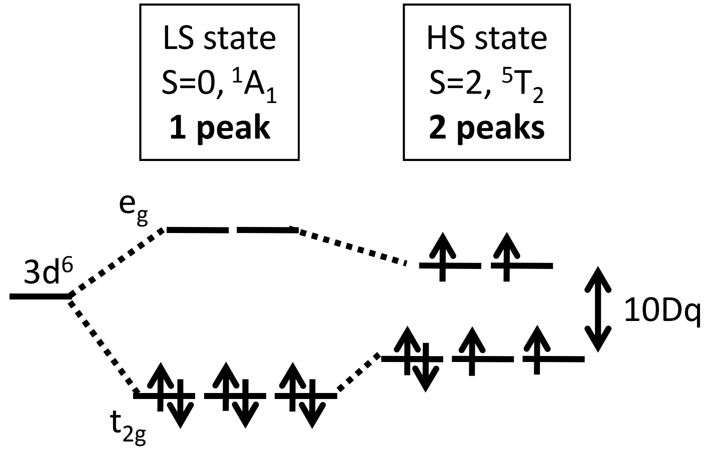
TR-Near Edge Structure

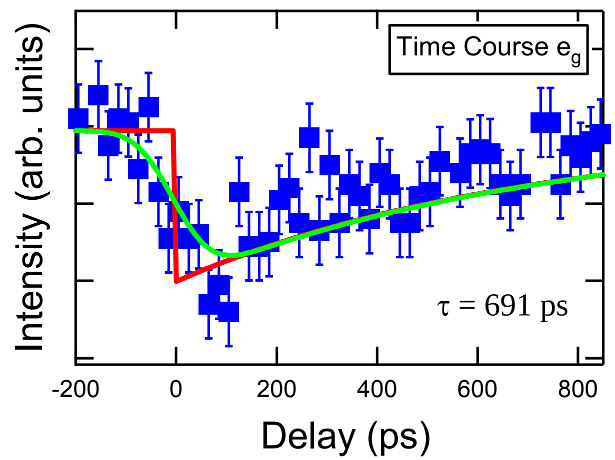




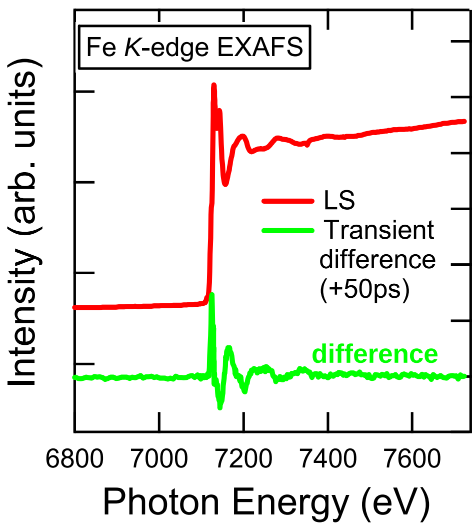
TR-XANES features in pre-edge region

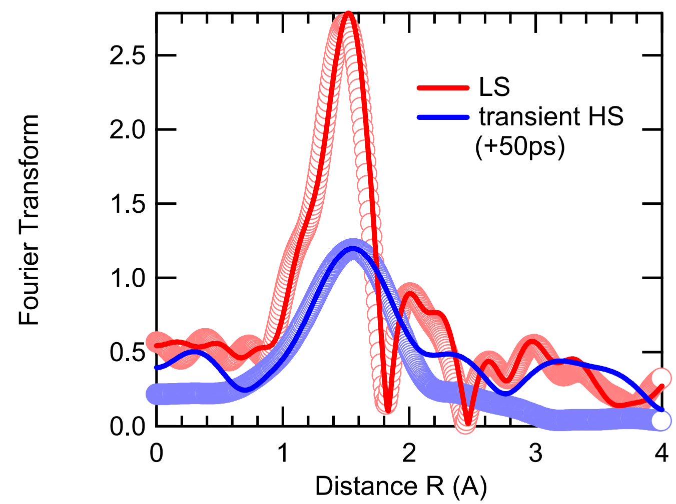






excited state EXAFS





EXAFS analysis summary

Spectrum	$R_{Fe\text{-}N}$ (Å)	σ^2 (Å^2)
LS	1.98(1)	0.001(1)
Photo-excited HS	2.15(2)	0.011(3)

photoinduced structural change: a molecular movie!

Low Spin State

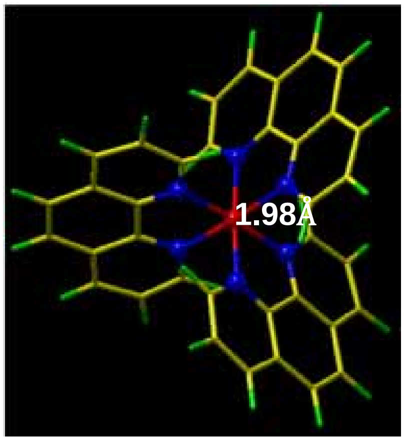
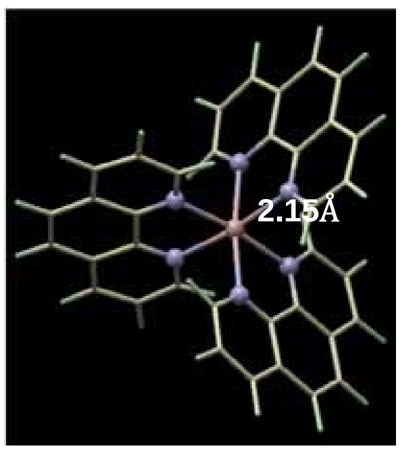
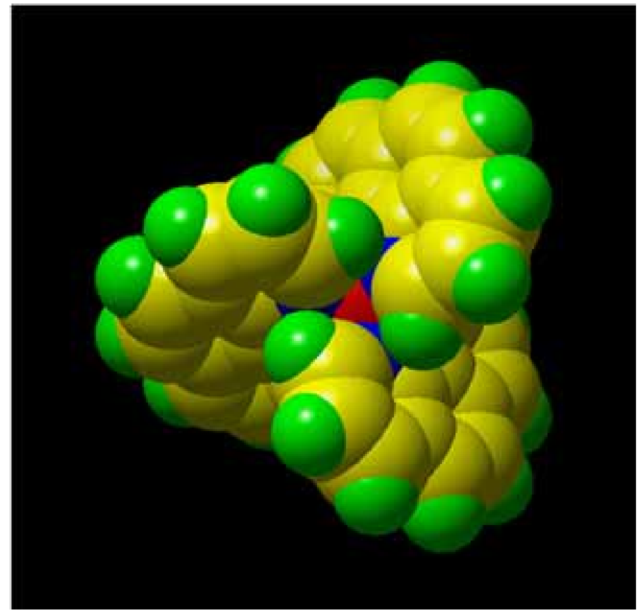
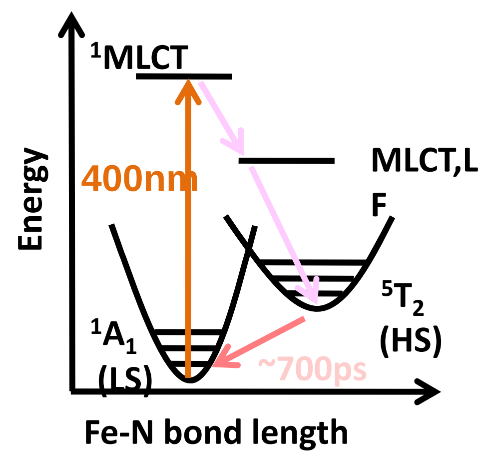


Photo-excited High Spin State

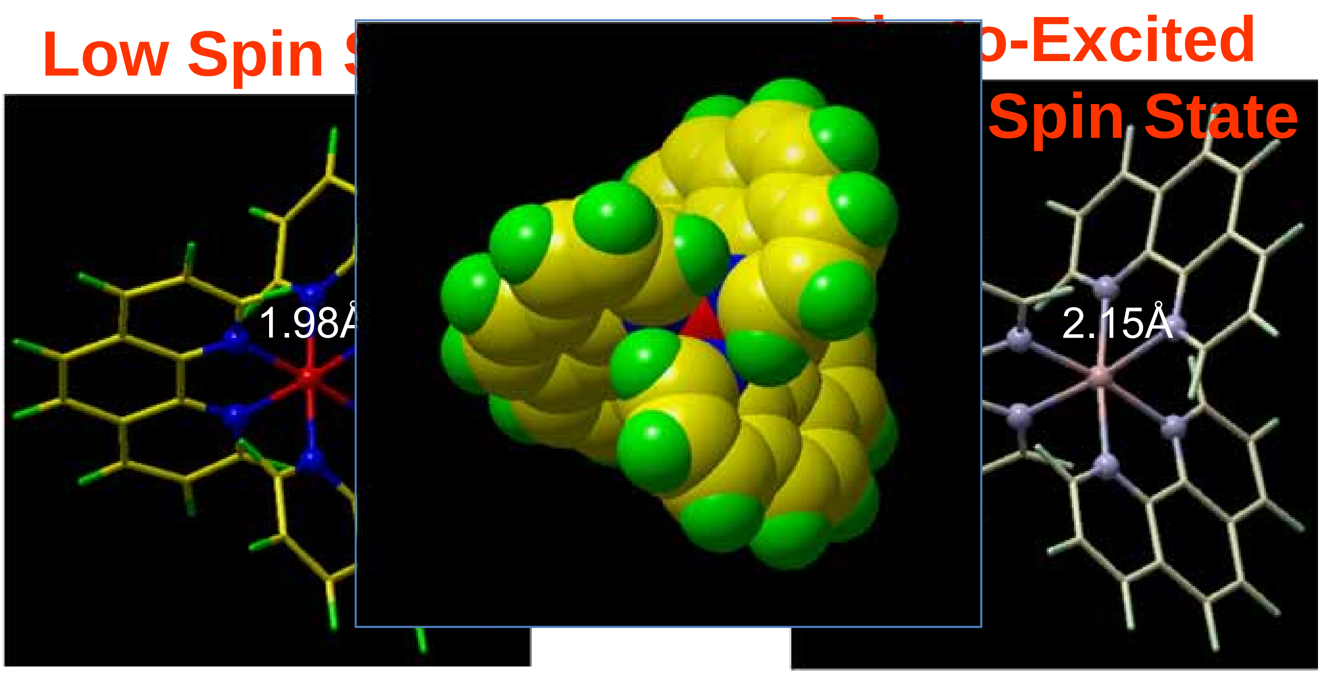






Nozawa *et al.* **J. Am. Chem. Soc., 132**, 61-63 (2010).

TR-XAFS - summary



- TR-XAFS provides spin, electronic and structural information of photo-induced states, which enables to produce molecular movies.

outline

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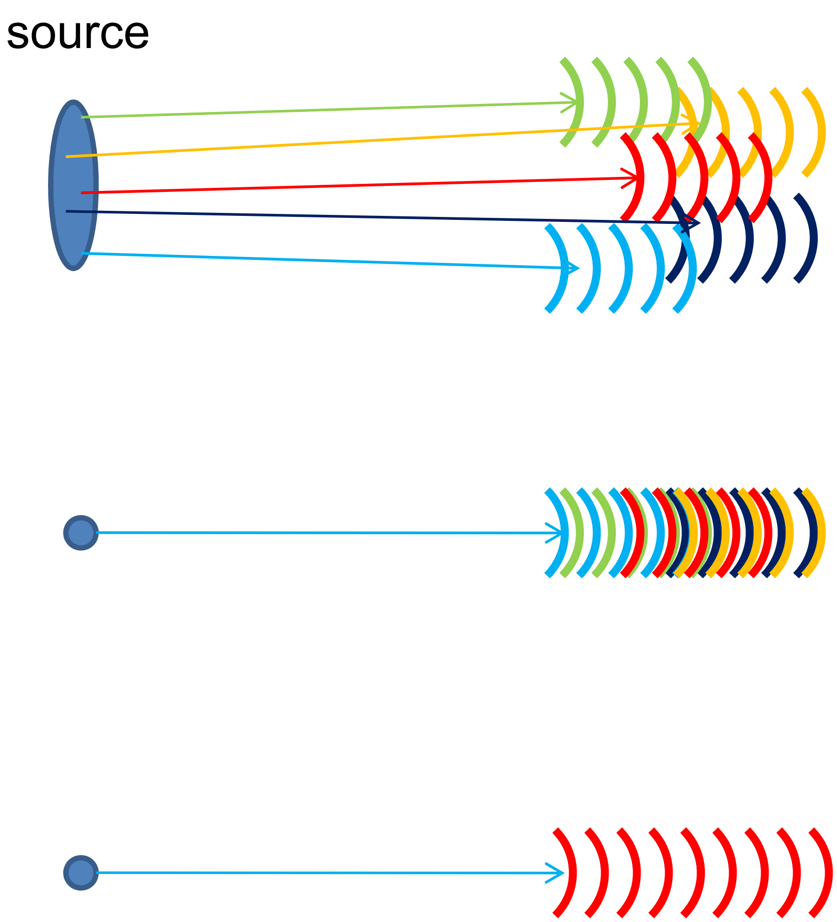
Evolution of the synchrotron sources



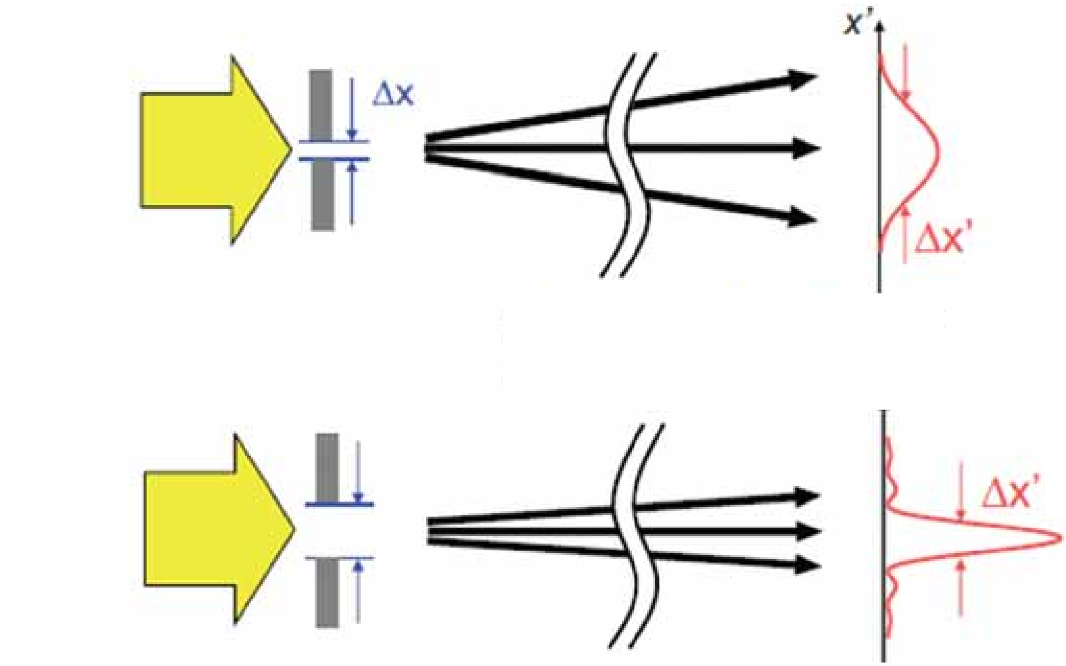
Case1: 3rd gen. synchrotron sources

Case2: ERL & SASE-XFEL
(Diffraction limit)

Case3: XFELO & seeded XFEL
(Fourier limit)

Diffraction Limit

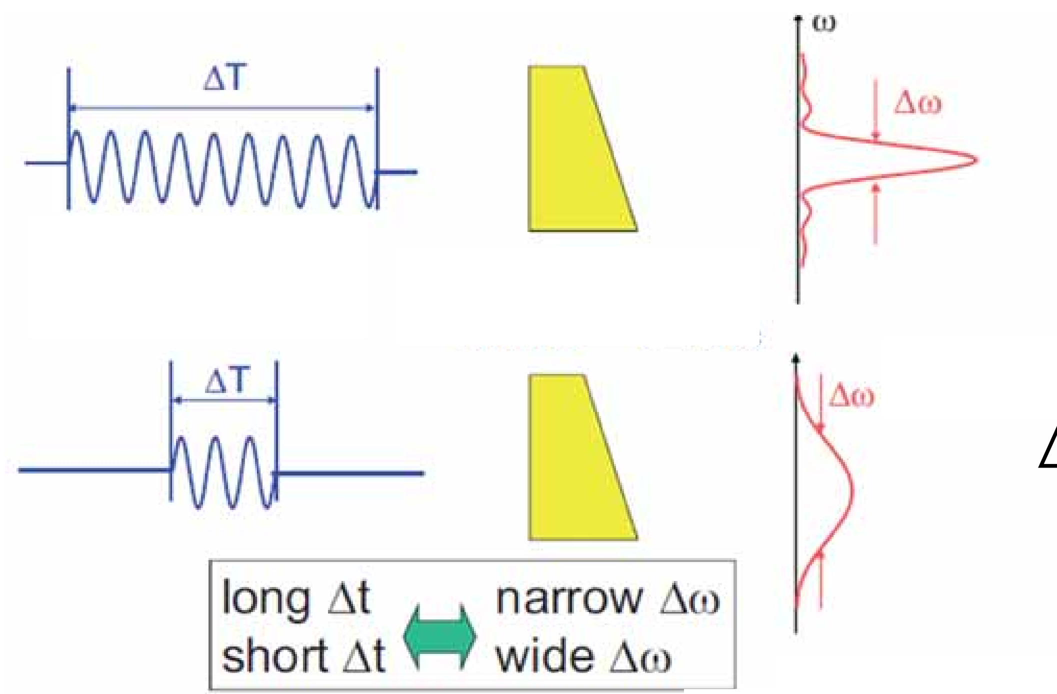
ERL & SASE-XFEL



$$\sigma_x \sigma_{x'} \geq \frac{\lambda}{4\pi}$$

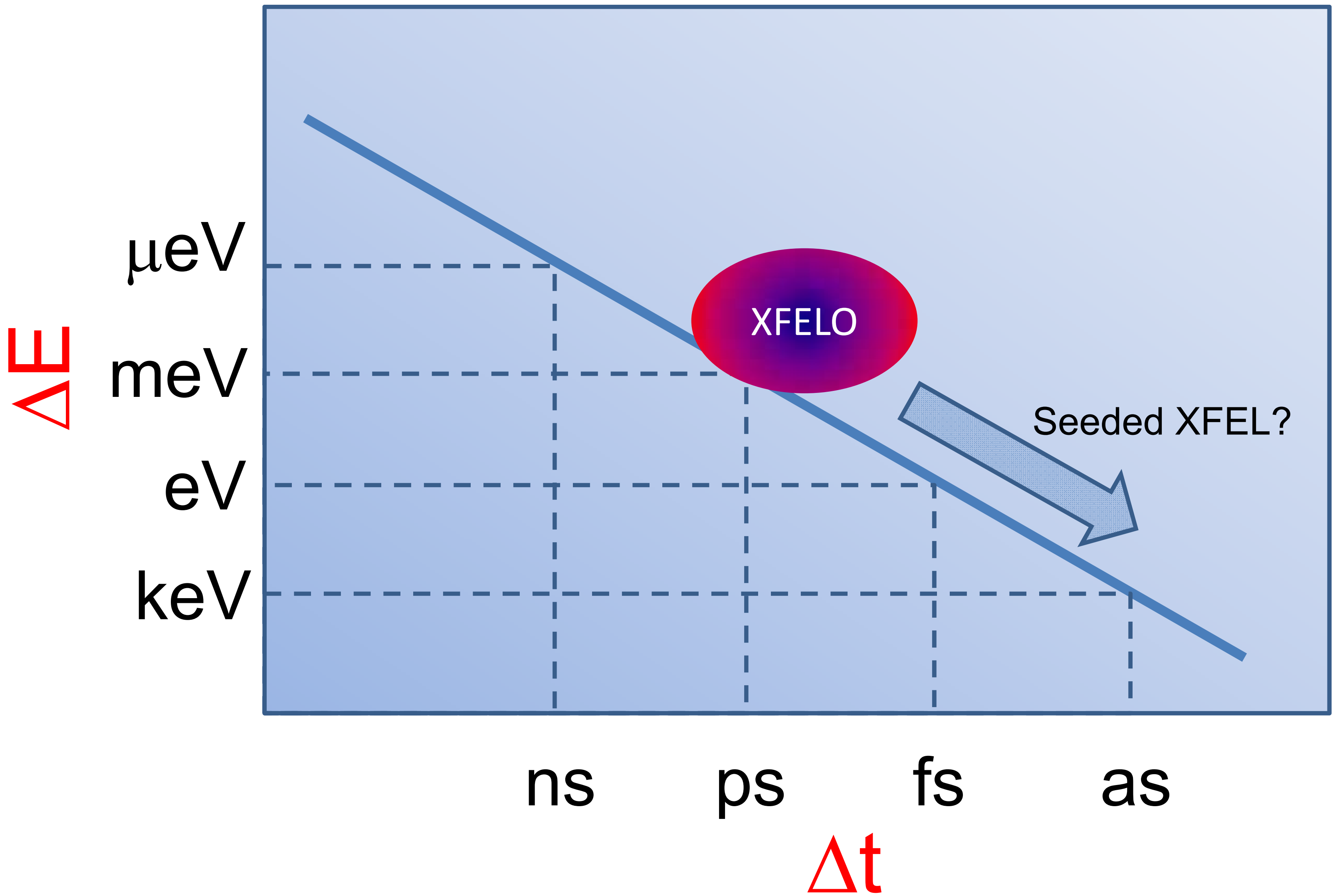
Fourier Limit

XFELO & seeded XFEL

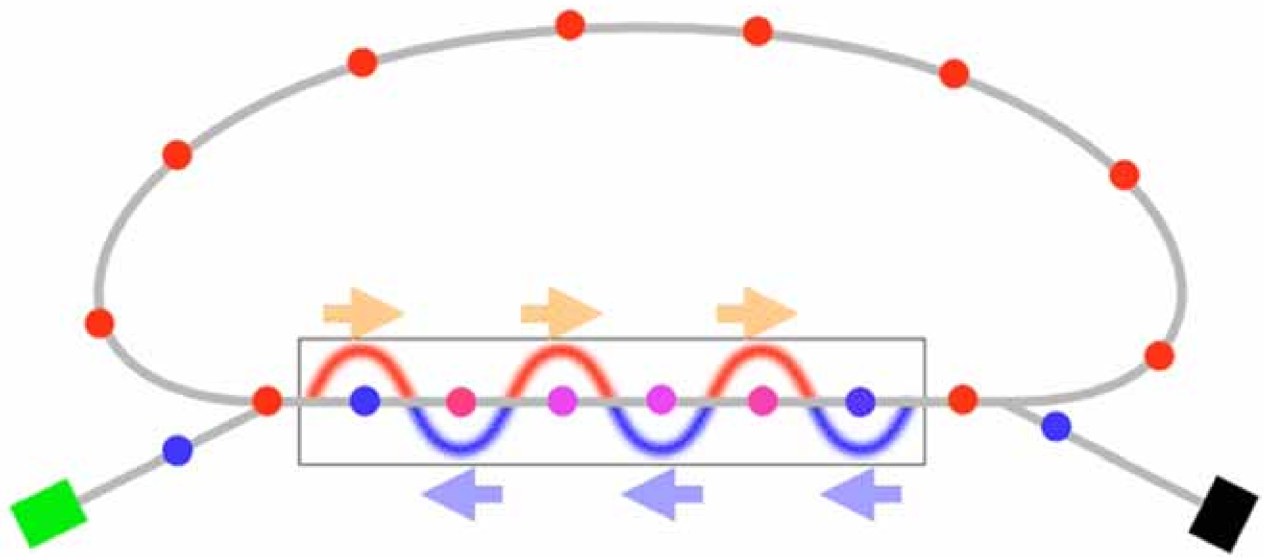


$$\Delta\omega\Delta t \geq \frac{h}{4\pi}$$

Fourier-limited X-ray



KEK Energy Recovery Linac (ERL) project



Linac based light source:

1) Diffraction-limited beam ***ε~15pmrad ~$\lambda/4\pi$***

2) Short pulse capability ***0.1~1 pico-second***

3) High repetition rate ***1.3 GHz***

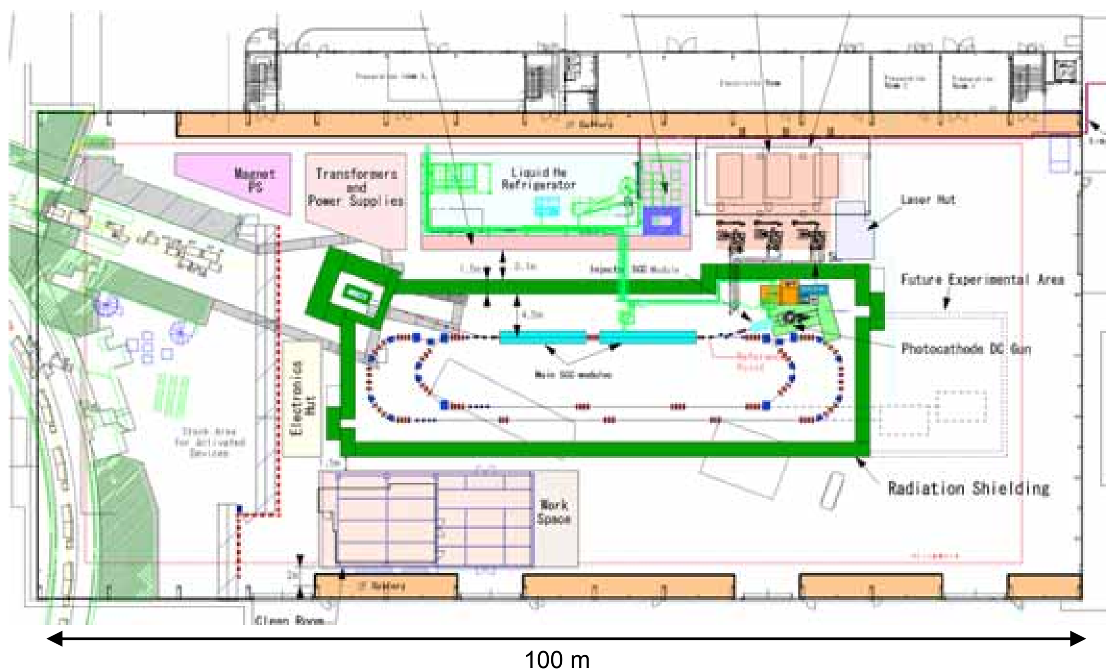
35-245MeV ERL test facility (Compact ERL)

- Plan and Status -

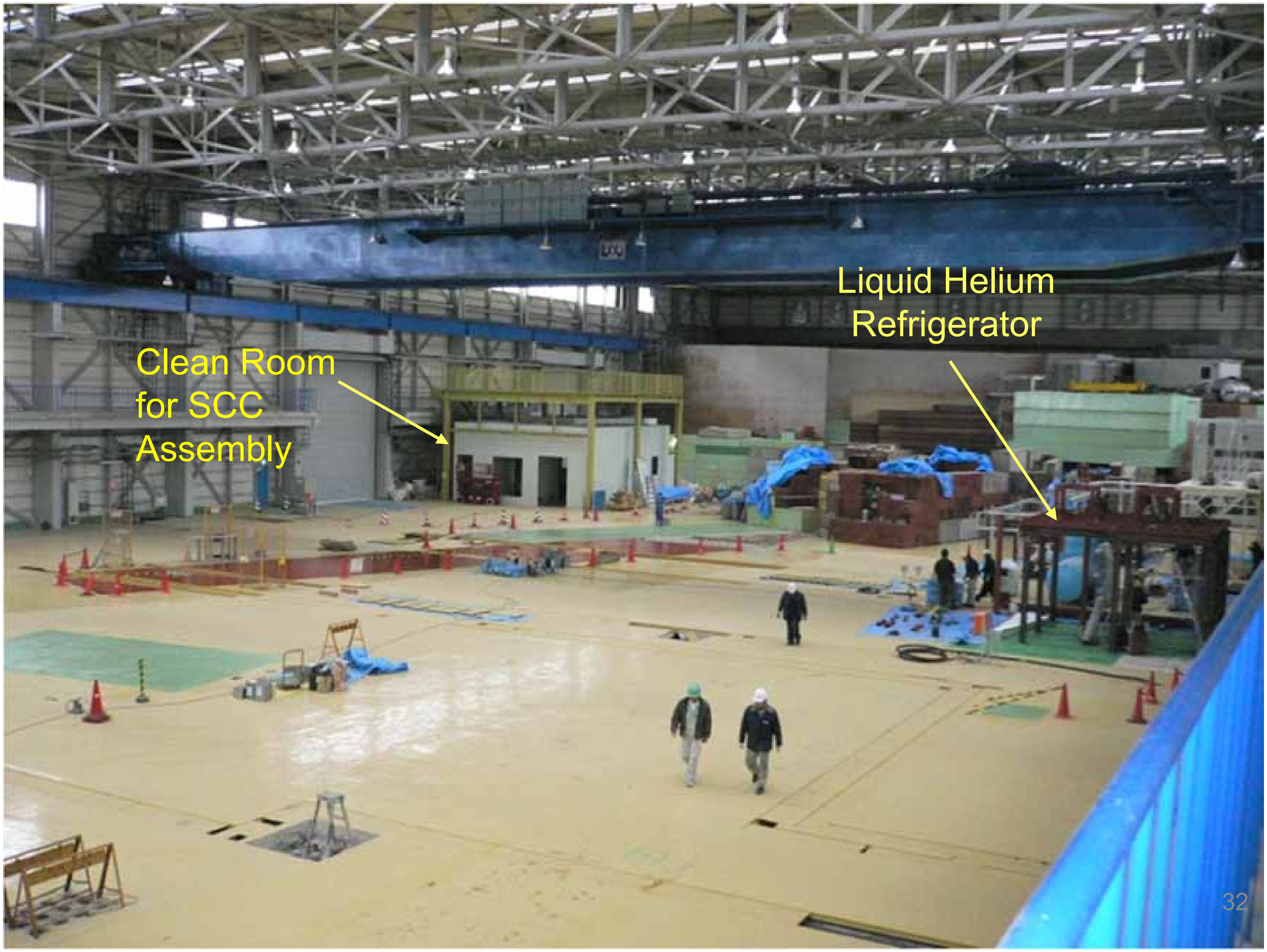
Compact ERL
for developing and demonstrating ERL technologies

Parameters of the Compact ERL

	Parameters
Beam energy	35 - 245 MeV
Injection energy	5 MeV
Average current	10 - 100 mA
Acc. gradient (main linac)	15 MV/m
Normalized emittance	0.1 - 1 mm·mrad
Bunch length (rms)	1 - 3 ps (usual) ~ 100 fs (with B.C.)
RF frequency	1.3 GHz

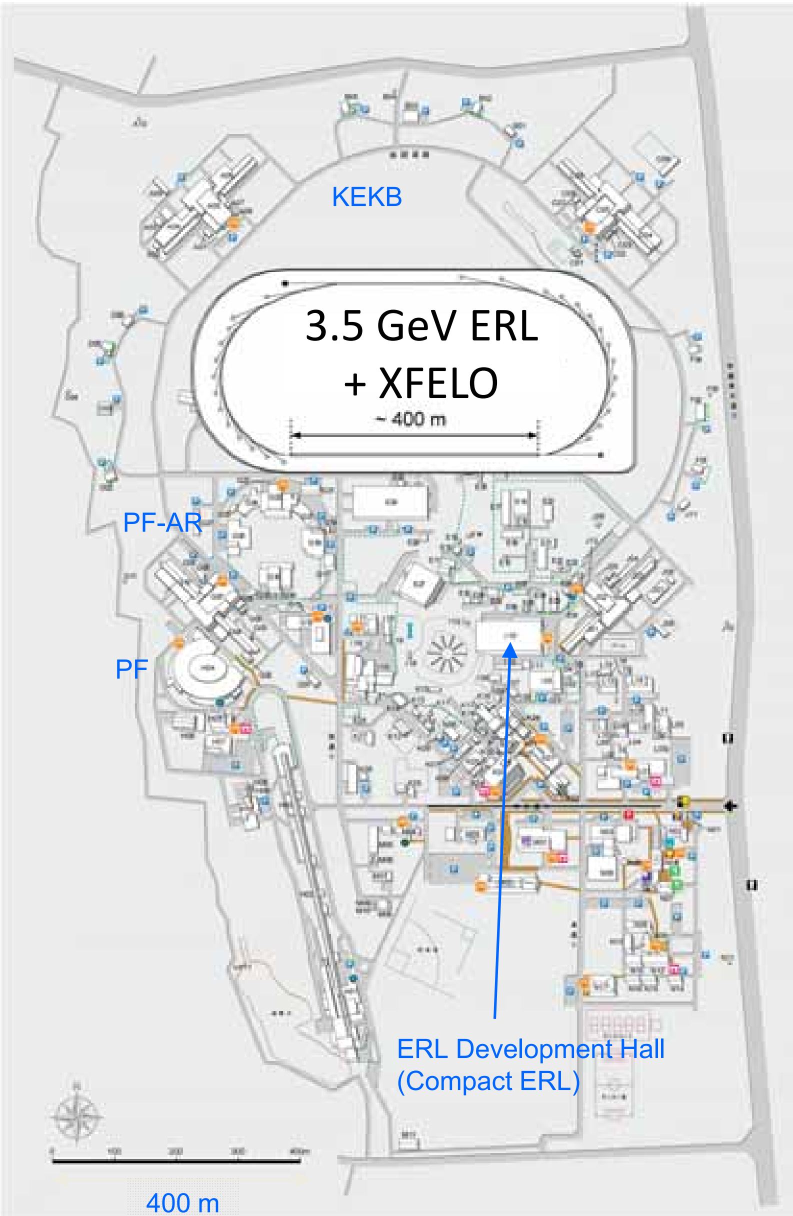


Recent View in the ERL Development Hall (EDH)



3.5GeV ERL (1st phase)
+ XFELO (2nd phase)

3.5GeV ERL Plan at KEK



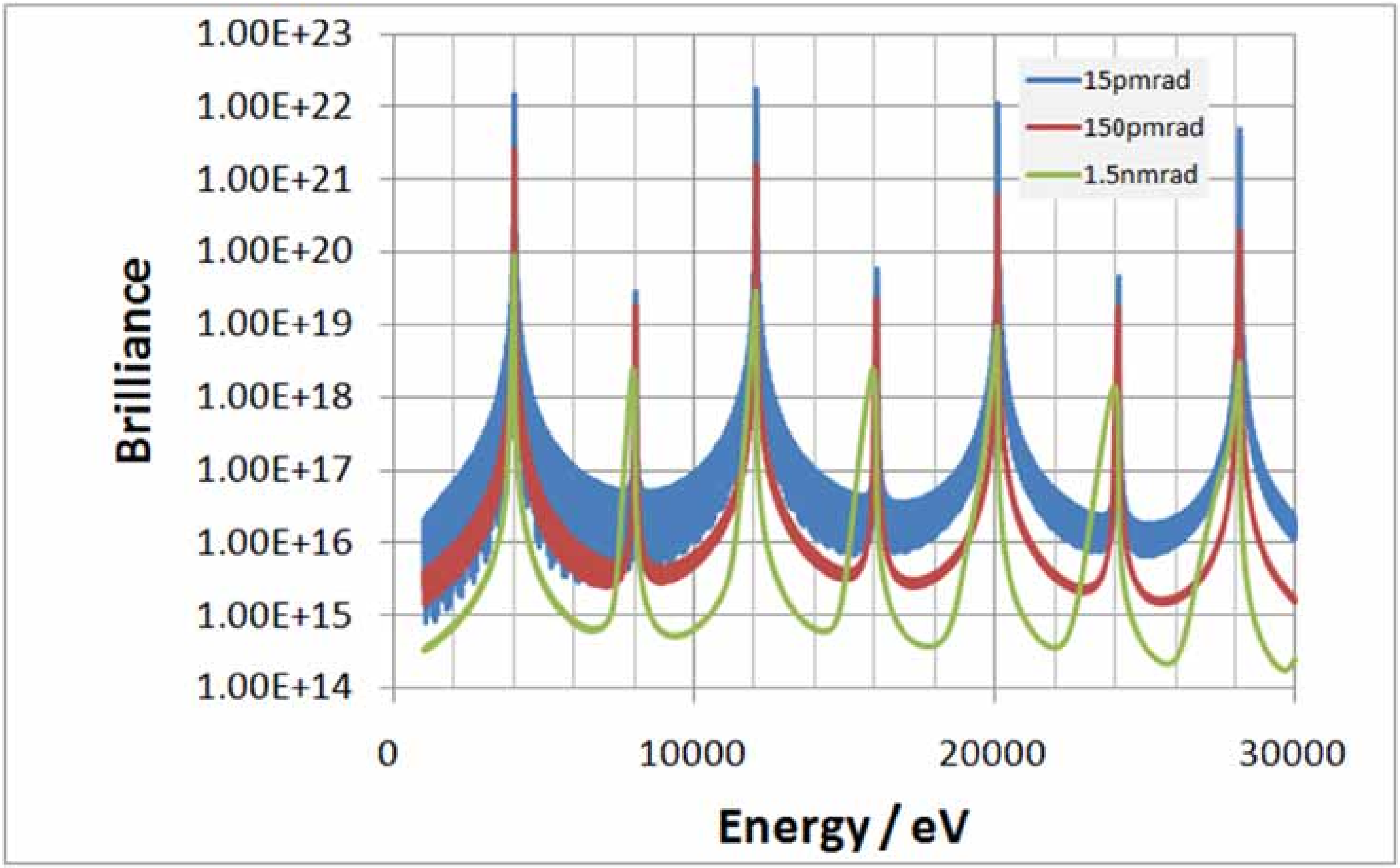
Parameters of the ERL

	Parameter
Beam energy	3.5 GeV
Average current	10 - 100 mA
Normalized emittance	0.1 – 1.0 mm·mrad
Energy spread (rms)	(0.5 - 2) $\times 10^{-4}$
Bunch length (rms)	1 - 3 ps (usual mode) ~ 100 fs (bunch compression)
RF frequency	1.3 GHz

Parameters of the light sources

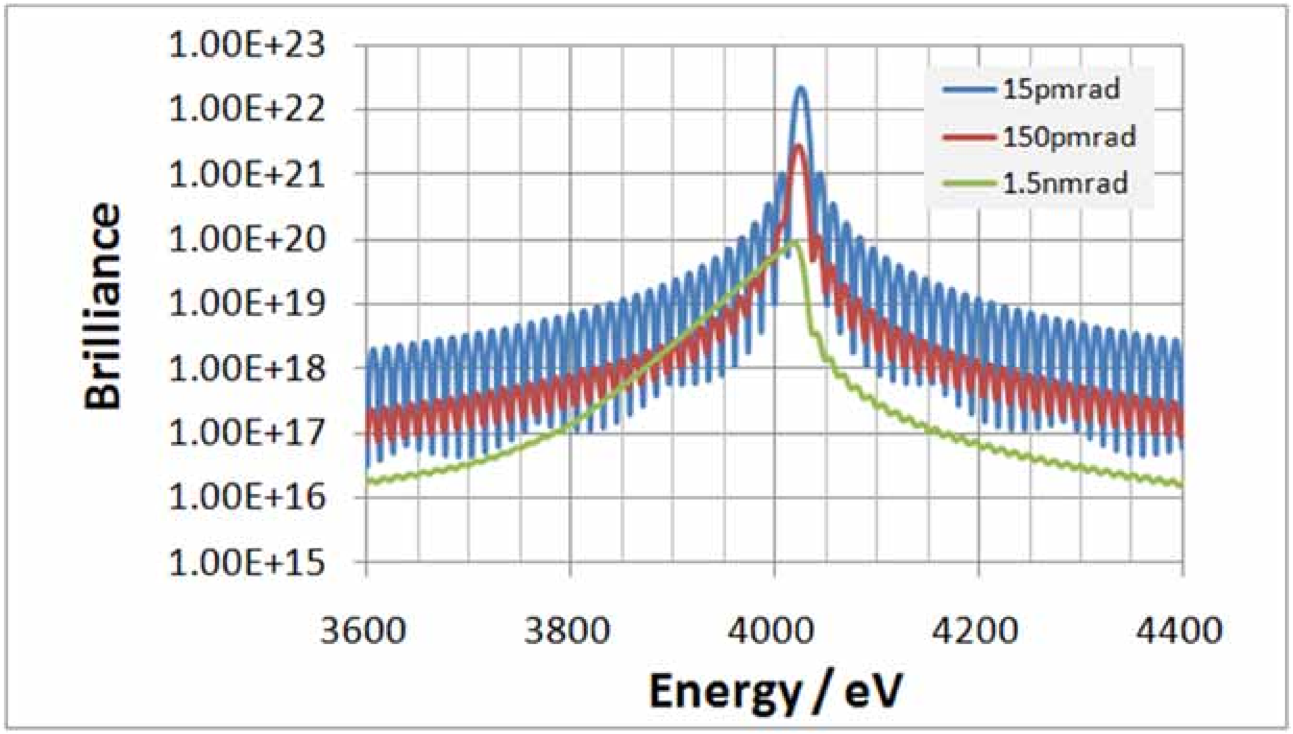
	Parameter
Spectral range	30 eV - 30 keV
Average brilliance from insertion devices	10^{21} - 10^{23} ph/s/mm^2/mrad^2/0.1%bw
Average flux	> 10^{16} phs/s/0.1%bw
Number of ID's	20 - 30

ERL undulator spectra
(with 15pmrad ~ 1.5nmrad natural emittance)



E=3.5GeV
I=100mA
$\beta x = \beta y$=5m
K=1.0
σ_E/E=4e-5
L=5m
λu=16mm

1^{st} harmonic of the undulator (@4024 eV)
(with 15pmrad ~ 1.5nmrad natural emittance)



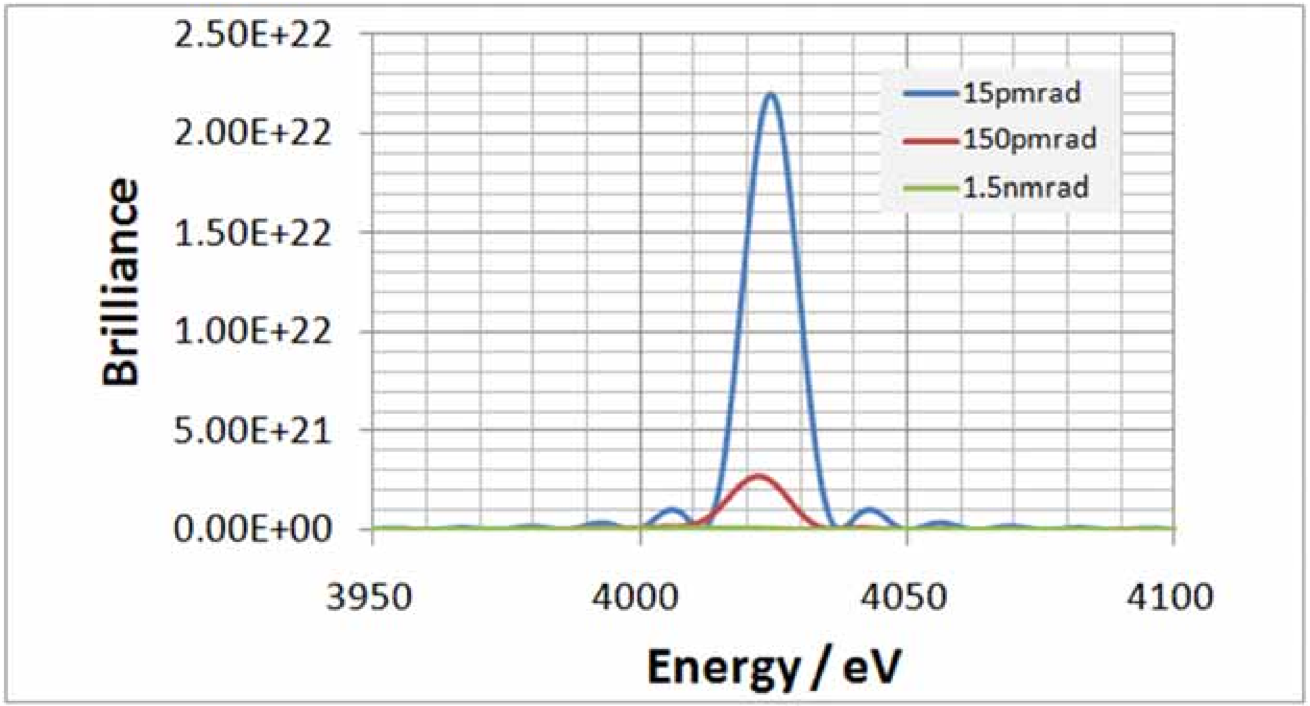
E=3.5GeV
I=100mA
$\beta x=\beta y=5m$
K=1.0
$\sigma_E/E=4e-5$
L=5m
$\lambda u=16mm$

Undulator radiation

$$I(\Delta\omega) \propto \left(\frac{\sin\left(\pi N \frac{\Delta\omega}{\omega}\right)}{\pi N \frac{\Delta\omega}{\omega}} \right)^2$$

1^{st} harmonic of the undulator (linear scale)

$\Delta E/E$ = 12 eV / 4024 eV = 0.0030

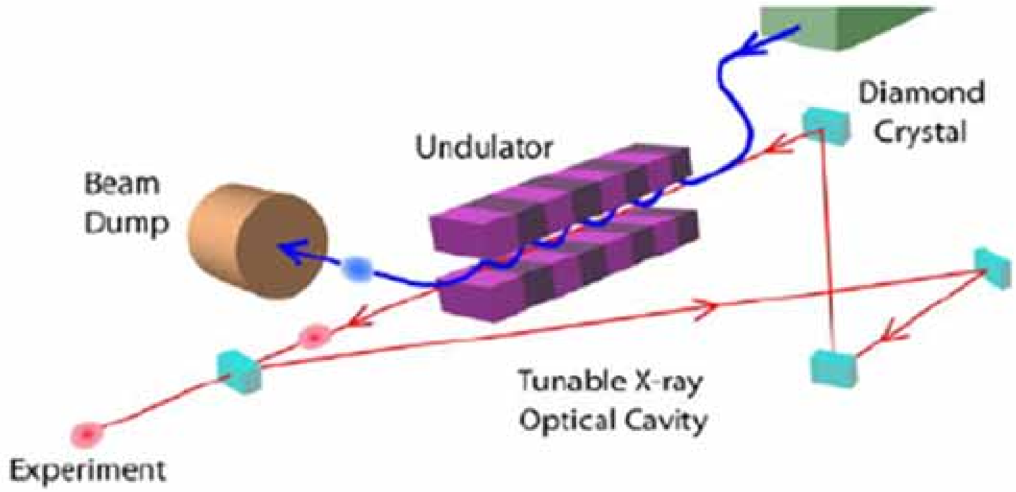


E=3.5GeV
I=100mA
$\beta x = \beta y$=5m
K=1.0
σ_E/E=4e-5
L=5m
λu=16mm

$\Delta\omega/\omega = 1/N$ N = 5000/16 = 313

1/N = 16/5000 = 0.0032

Hard X-Ray FEL Oscillator



- Store an X-ray pulse in a Bragg cavity→ multi-pass gain & spectral cleaning
- Provide meV bandwidth ($\Delta\omega/\omega \sim 10^{-7}$)
- MHz pulse repetition rate→ high average brightness

Originally proposed in 1984 by Collela and Luccio and resurrected in 2008 (KJK, S. Reiche, Y. Shvyd'ko, PRL 100, 244802 (2008)

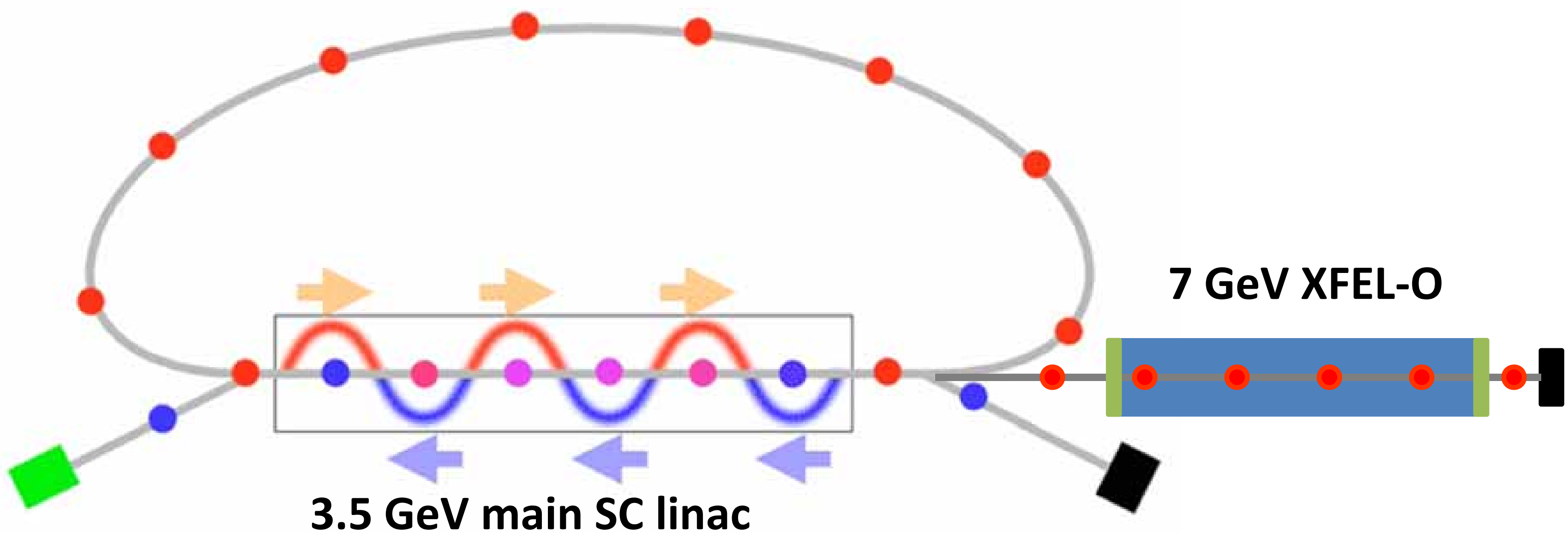
Courtesy of K.-J. Kim

Low emittance and high rep rate of ERL matches the specs of XFEL Oscillator (XFELO)

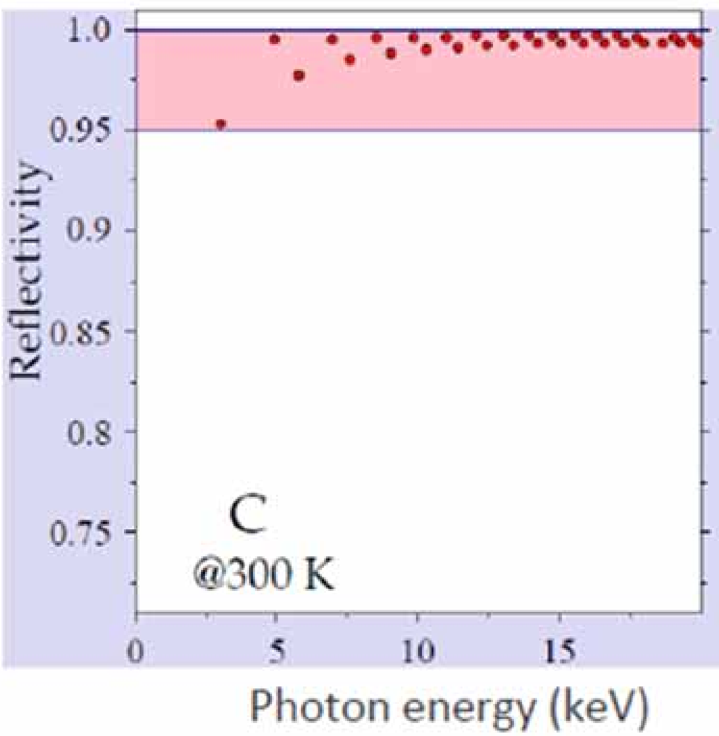
K.-J. Kim et al. PRL (2008) 100, 244802

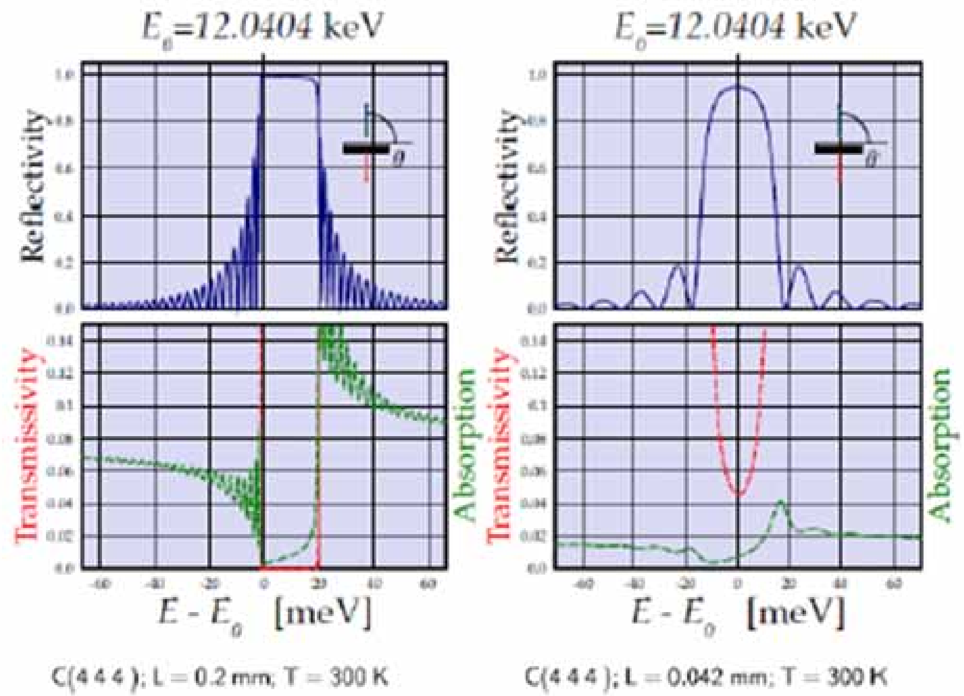
- **Electron beam:**
  - **Energy 7 GeV**
  - **Bunch charge ~ 25 - 50 pC**
  - **Bunch length (rms) 0.1 - 1.0 ps**
  - **Normalized rms emittance < 0.2 - 0.3 mm-mr**
  - **Energy spread (rms) ~ 2×10^{-4}**
  - **Constant bunch rep rate @ ~1 MHz**
- **Undulator:**
  - **L_u= 20 - 60 m, λ_u=2.0 cm, K=1.0 - 1.5**
- **Optical cavity:**
  - **2- or 4- diamond crystals and focusing mirrors**
  - **Total round trip reflectivity > 50 - 85 %**
- **XFELO output:**
  - **5 keV - 25 keV**
  - **Bandwidth: $\Delta\omega/\omega$ ~ 1×10^{-7} , pulse length (rms) = 80- 500 fs**
  - **# photons/pulse ~ 1×10^{9}**

Energy Recovery Linac (ERL) and XFEL Oscillator



Diamond backscattering : High reflectivity and narrow bandwidth

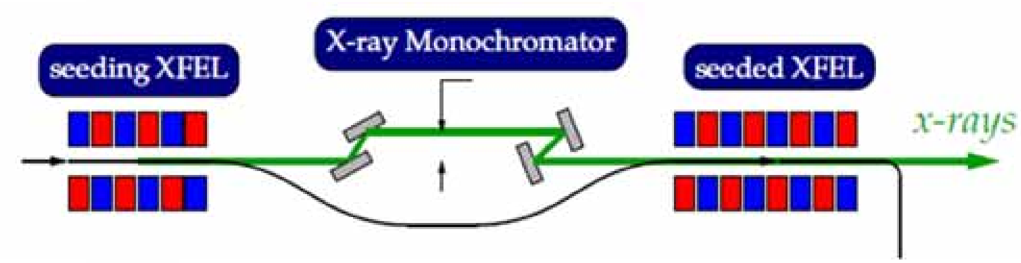


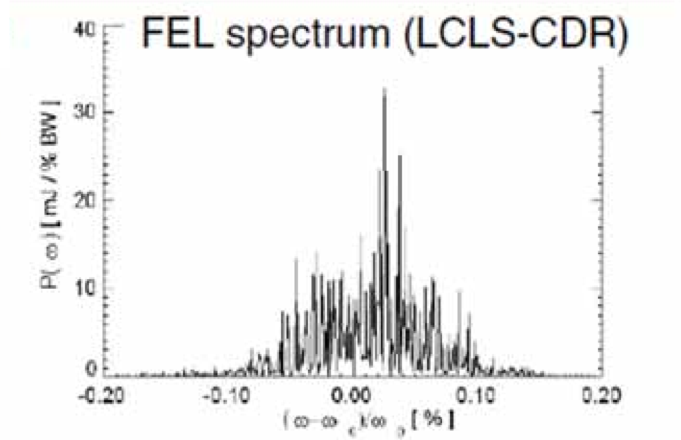


Courtesy of Yuri Shvyd'ko

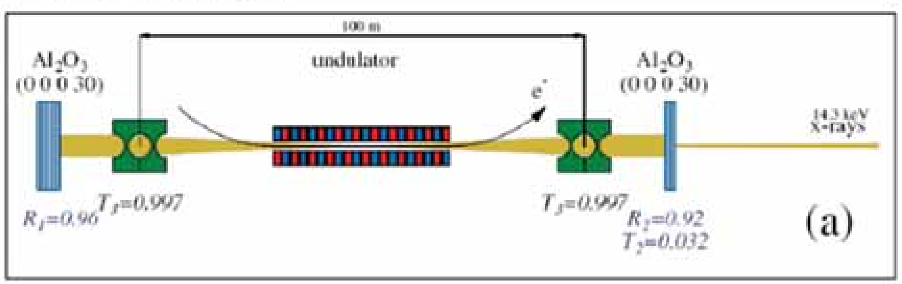
Seeded XFEL & XFELO

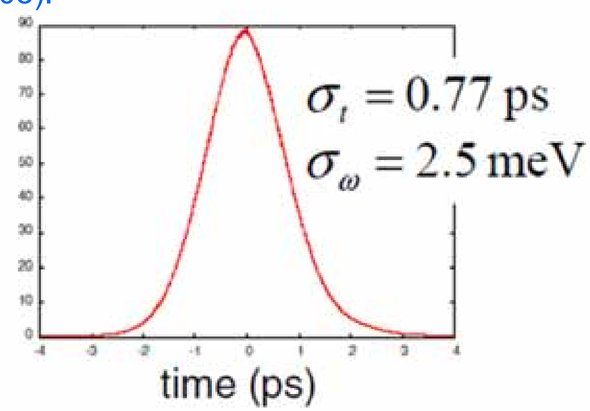
Seeded XFEL





XFEL- Oscillator cf. K.-J. Kim et al., PRL 100, 244802 (2008).

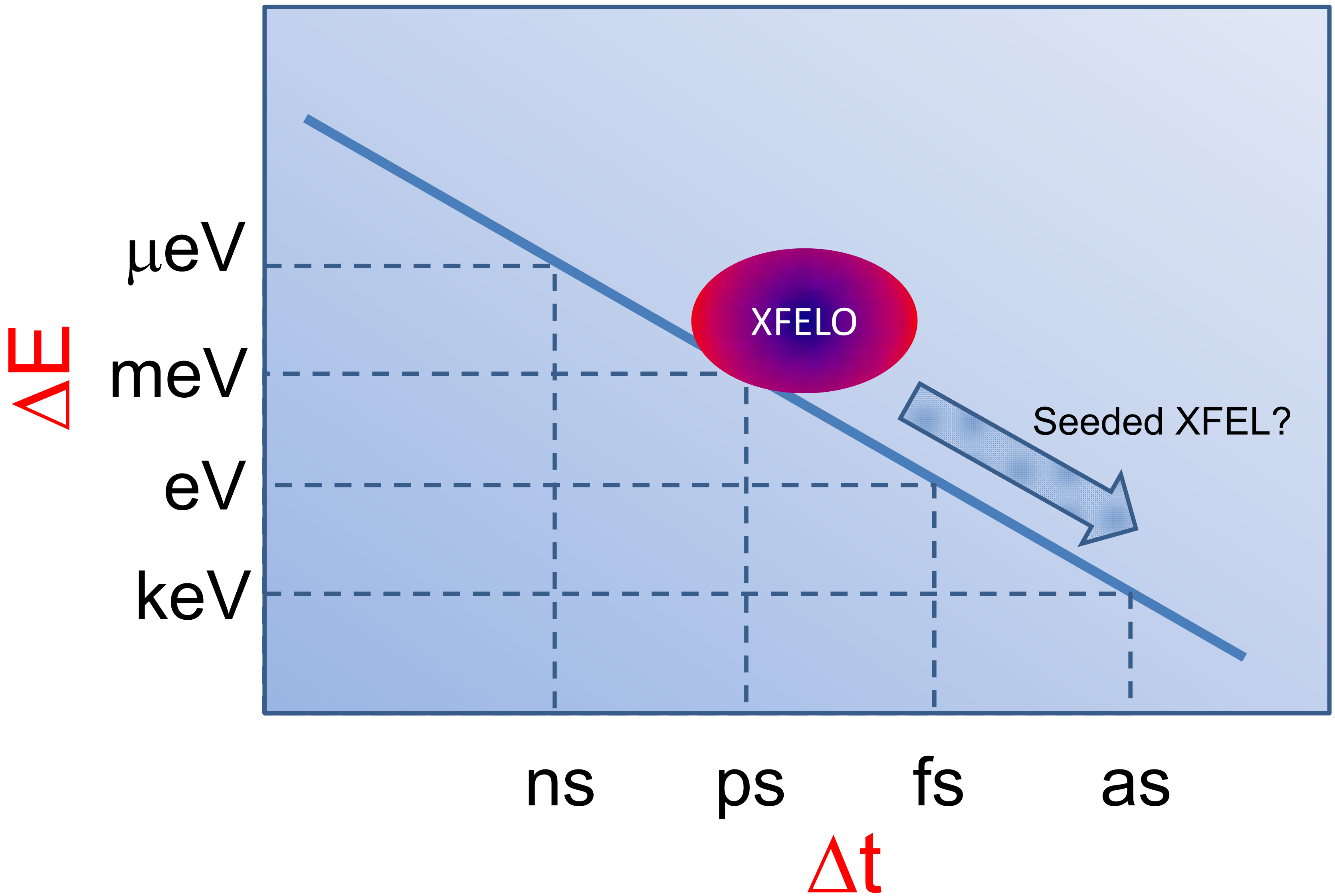




outline

- Time-domain X-ray science
  - with Storage Ring (Photon Factory Advanced ring, KEK)
- Current status of Energy Recovery Linac (ERL) project at KEK
  - 35-245MeV ERL test facility (under construction)
  - 3.5GeV ERL + XFEL Oscillator (not approved)
- Towards Fourier-limited X-ray Science with XFEL-O and seeded XFEL
  - Inelastic X-ray scattering
  - Nonlinear X-ray Optics
  - Two-photon correlation spectroscopy
  - Transient grating
- Summary

Fourier-limited X-ray



1. inelastic X-ray scattering

Current High Resolution IXS @ APS, ESRF, SPring-8

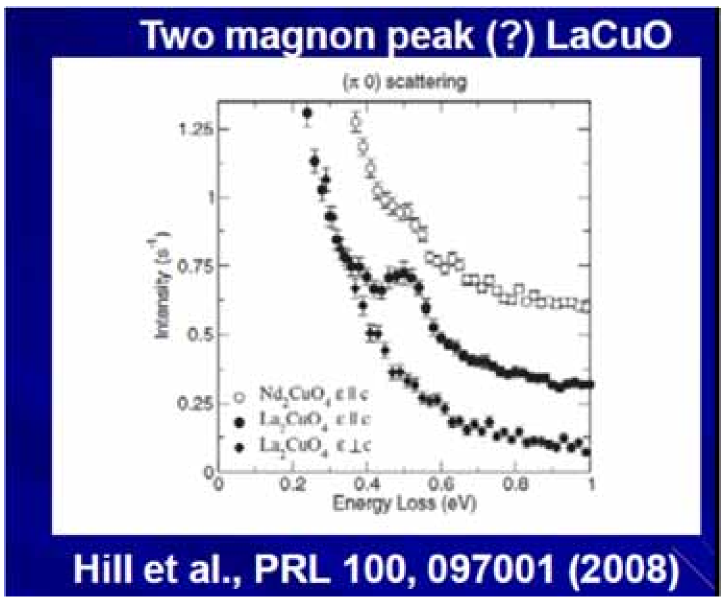
10^9-10^{10} photons/sec, ΔE~1meV

XFELO X-ray beam characteristics

1×10^9 photons/pulse @ 1MHz

1×10^{15} photons/sec

$\Delta\omega/\omega \sim 10^{-7}$



Ideal for IXS, NRS, HXPES, etc…

APS XFELO Workshop 2010
Presentation by Clement Burns
(Western Michigan Univ.)

2. Nonlinear X-ray Optics

- **Quantitative and systematic studies will require Fourier-limited X-rays**
- **Sum- & difference-frequency mixing applications**
- **Parametric down-conversion**
  - X (pump) → X' (signal) + EUV or SX (idler)

PRL 98, 244801 (2007) PHYSICAL REVIEW LETTERS week ending 15 JUNE 2007

Interference between Compton Scattering and X-Ray Parametric Down-Conversion

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RIKEN SPring-8 Center, 1-1-1 Koto, Sayo-cho, Sayo-gun, Hyogo 679-5148 Japan
(Received 15 December 2006; published 14 June 2007)

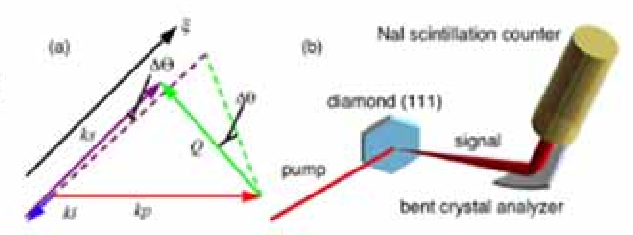
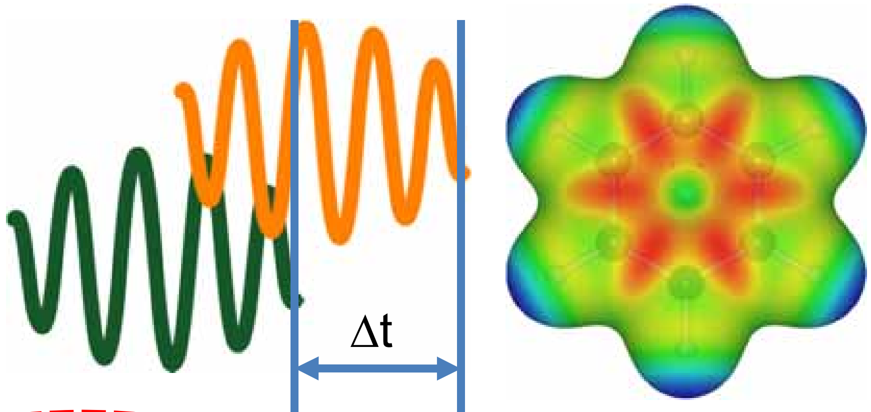
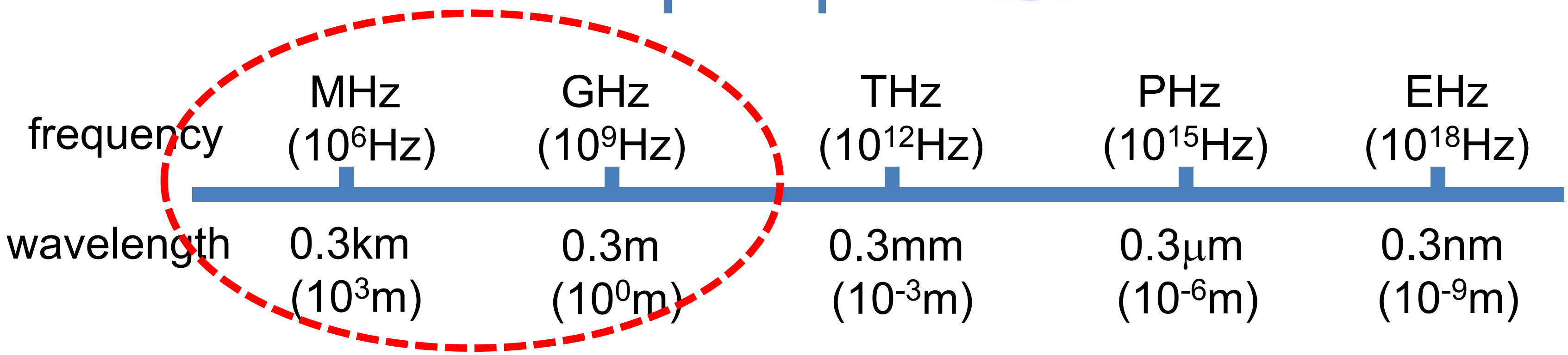


FIG. 1 (color online). (a) The phase-matching geometry used in the theoretical calculation and the experiment. Dashed lines indicate the geometry for $E_i = 0$, i.e., the Bragg diffraction. (b) Schematic view of the experimental setup.

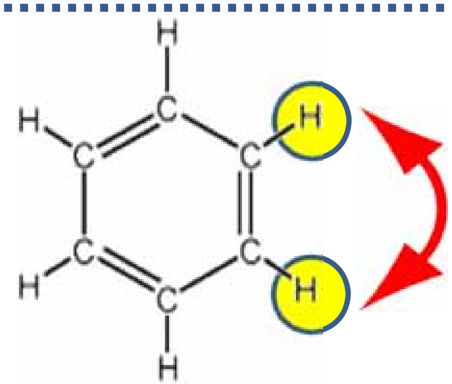
3. two-photon correlation spectroscopy (1) in radio wave domain





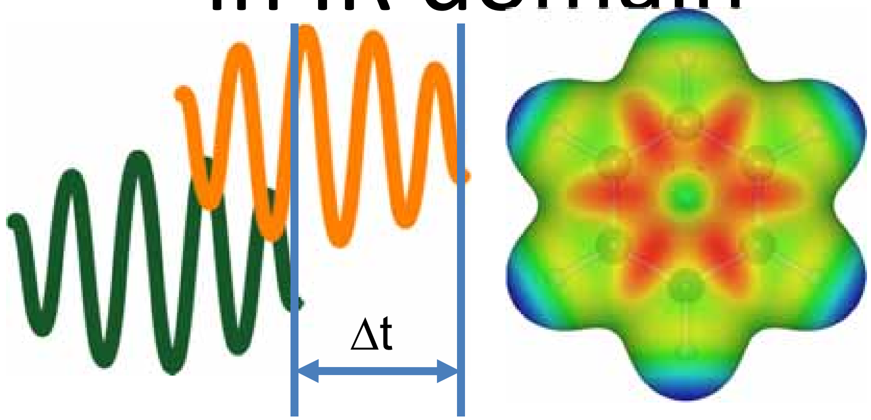
Radio wave domain

Multi-dimensional NMR



Correlation of nuclear magnetic spin

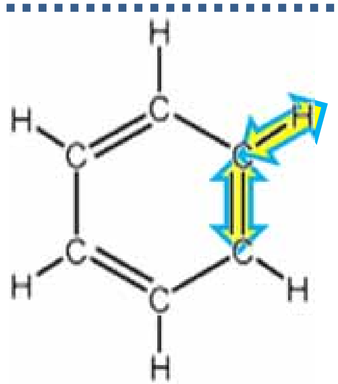
two-photon correlation spectroscopy (2) in IR domain



frequency	MHz (10^6Hz)	GHz (10^9Hz)	THz (10^{12}Hz)	PHz (10^{15}Hz)	EHz (10^{18}Hz)
wavelength	0.3km (10^3m)	0.3m (10^0m)	0.3mm (10^{-3}m)	0.3μm (10^{-6}m)	0.3nm (10^{-9}m)

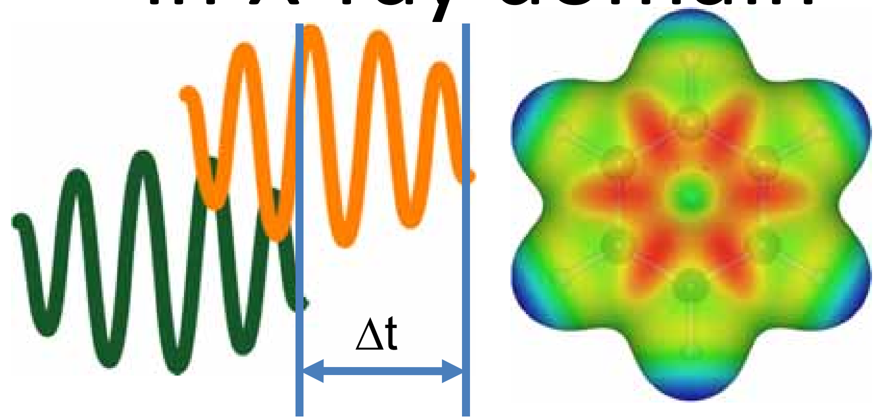
IR region

Multi-dimensional IR spectroscopy (photon echo)



Correlation of vibrational modes

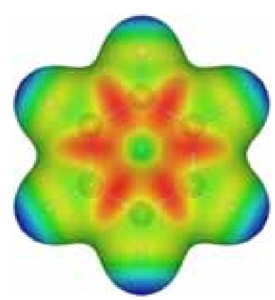
two-photon correlation spectroscopy (3) in X-ray domain



	MHz	GHz	THz	PHz	EHz
frequency	(10^6Hz)	(10^9Hz)	(10^{12}Hz)	(10^{15}Hz)	(10^{18}Hz)
wavelength	0.3km (10^3m)	0.3m (10^0m)	0.3mm (10^{-3}m)	0.3μm (10^{-6}m)	0.3nm (10^{-9}m)

X-ray region

Multi-dimensional X-ray spectroscopy

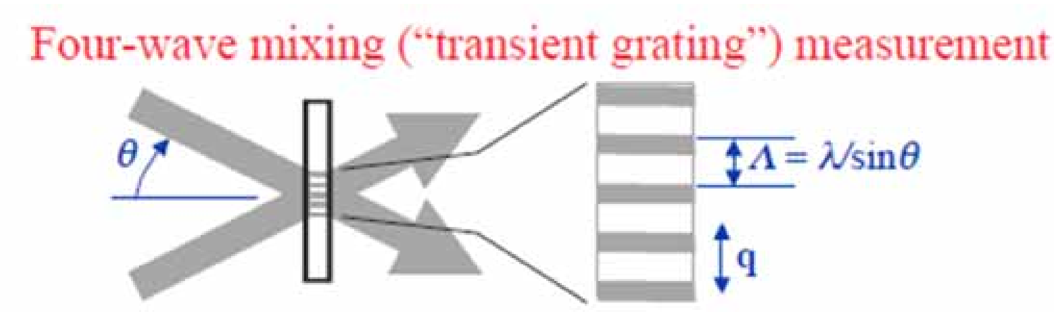


Correlation of electronic states, Wave packet motion?

4. Transient grating

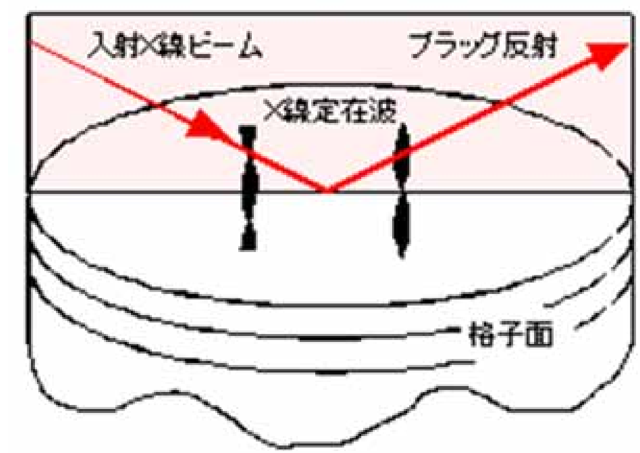
Transient X-ray standing wave without perfect crystal

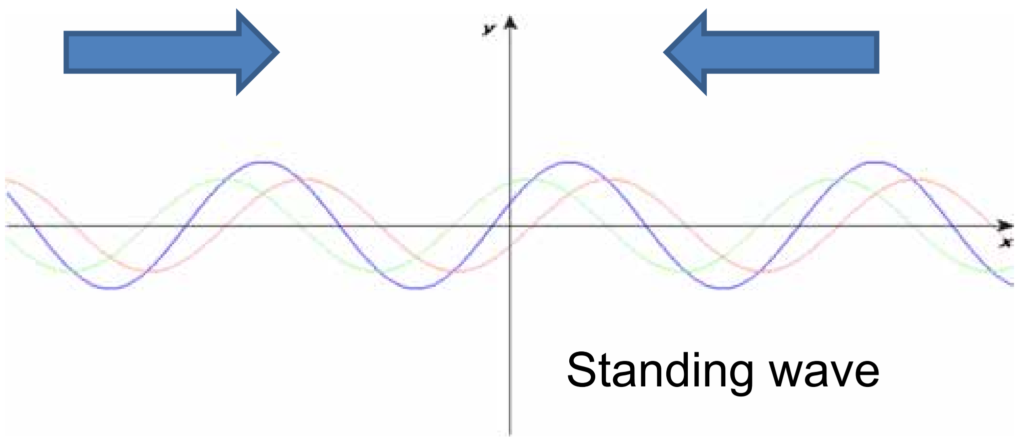
Transient grating with fully coherent X-ray



Proposed by Keith Nelson

X-ray standing wave

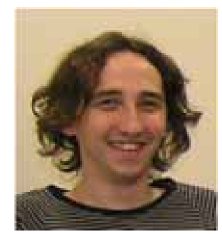




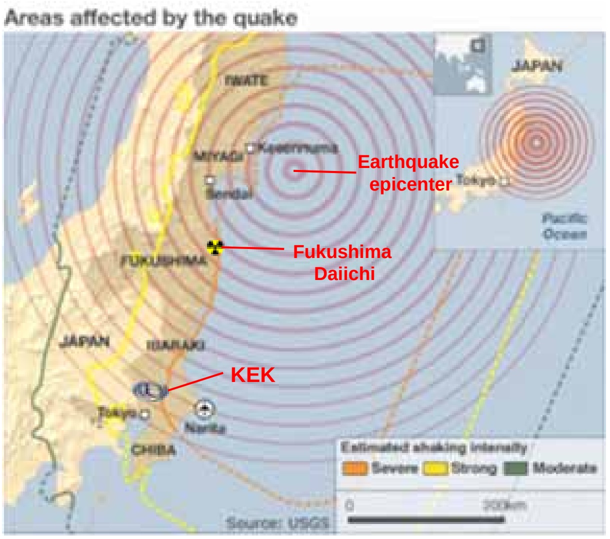
Summary

- SC Linac-based light source enables electron beam with high rep rate and low emittance suitable for Fourier-limited X-ray sources.
- Fourier-limited X-ray may open new X-ray applications in inelastic X-ray scattering, nonlinear X-ray optics, two-photon correlation spectroscopy and transient grating.

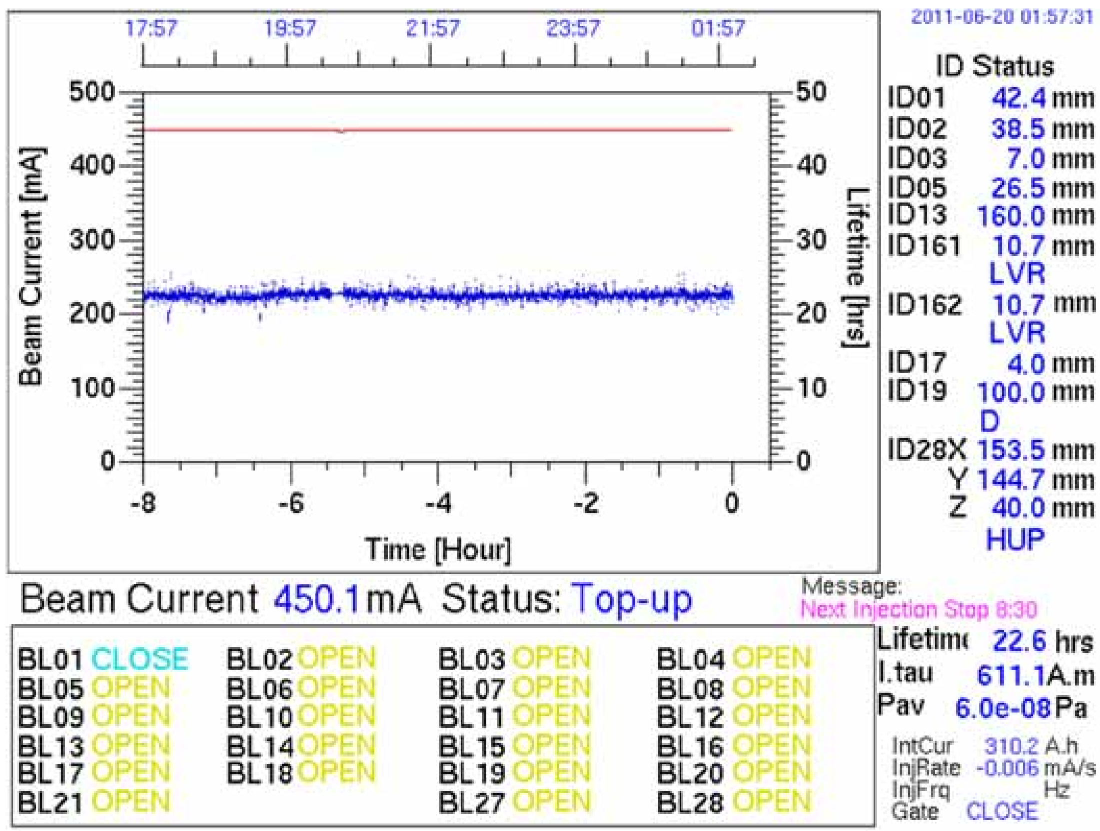
members @ Beam Line NW14A, KEK

Shunsuke Nozawa (KEK)		Tokushi Sato (KEK)	
Manabu Hoshino (TITECH)		Ayana Tomita (KEK)	
Matthieu Chollet (→APS)		Laurent Guérin (→Univ. Rennes 1)	
Hirohiko Ichikawa (JST)		Shin-ya Koshihara (TITECH)	

Recovery from the earthquake…



Damages at KEK
March 11, 2011



Photon Factory now operating!
Top-up mode
June 20, 2011

Thank you
for your attention