The Abdus Salam International Centre for Theoretical Physics

2369-23

CIMPA/ICTP Geometric Structures and Theory of Control

1 - 12 October 2012

New trends for warm dense matter research works and their applications

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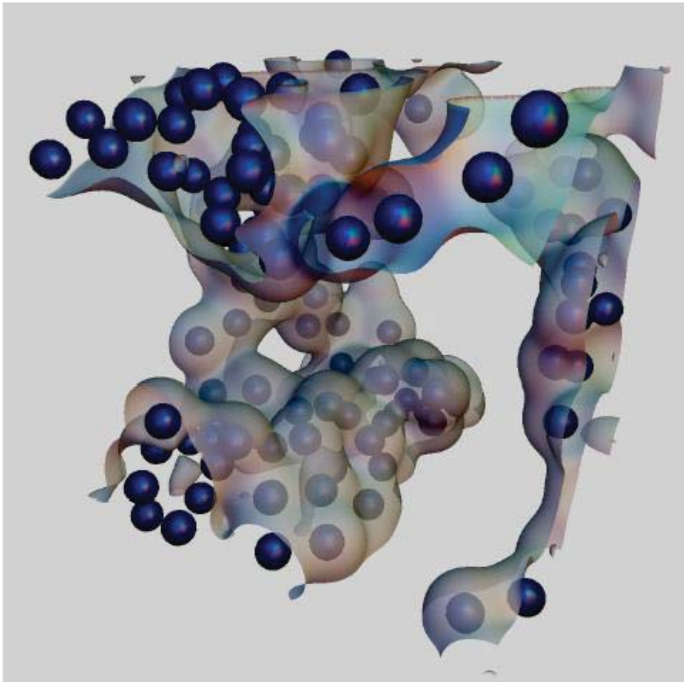
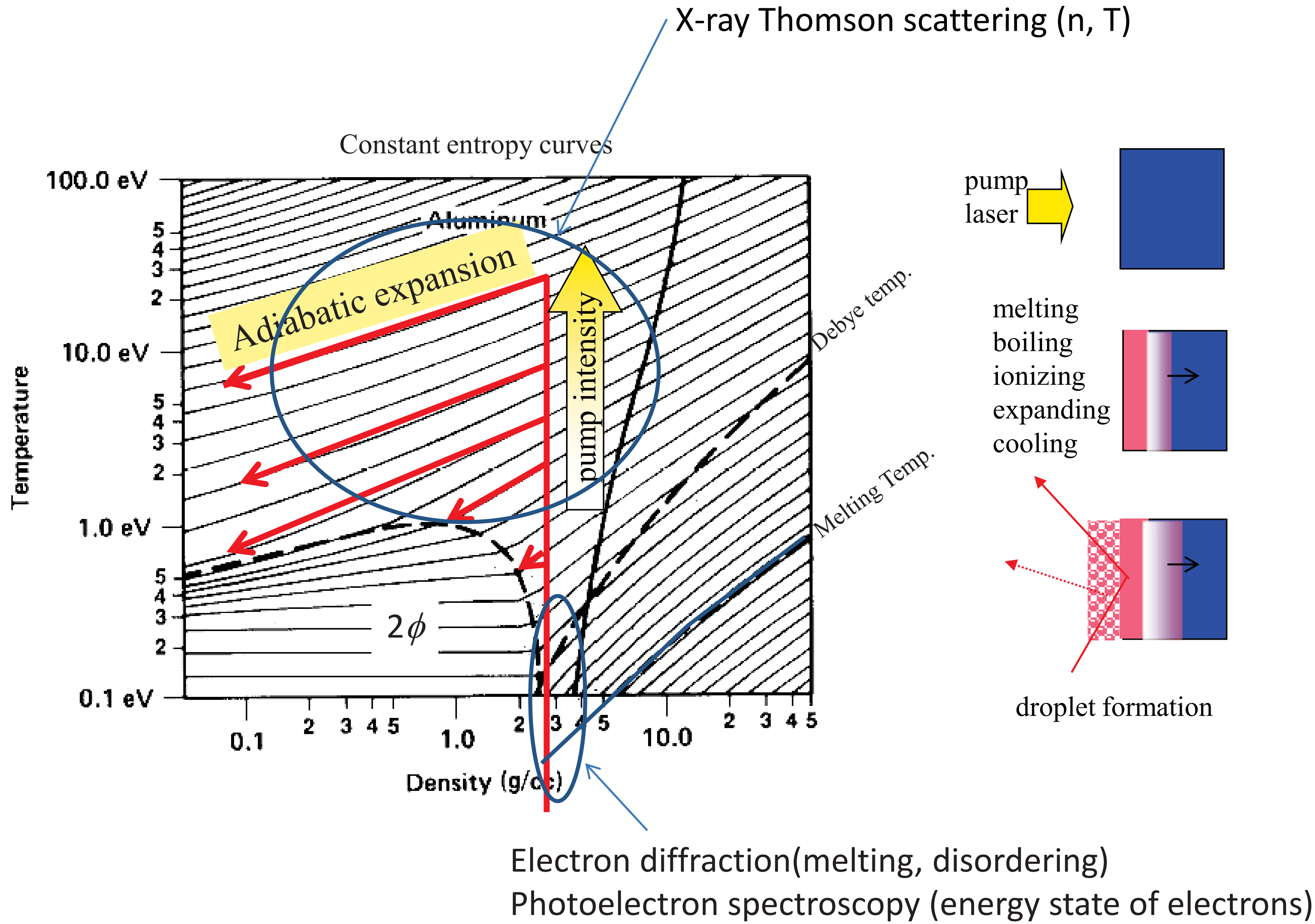
New trends for warm dense matter research works and their applications

We should measure directly the energy density state of electrons, disordering of ions, transport coefficient (electron, diffusion, thermal….), sound velocity, viscosity, and specific heat.



QMD simulation view of wdm Al, Michael Desjarlais, 2008 WDM school

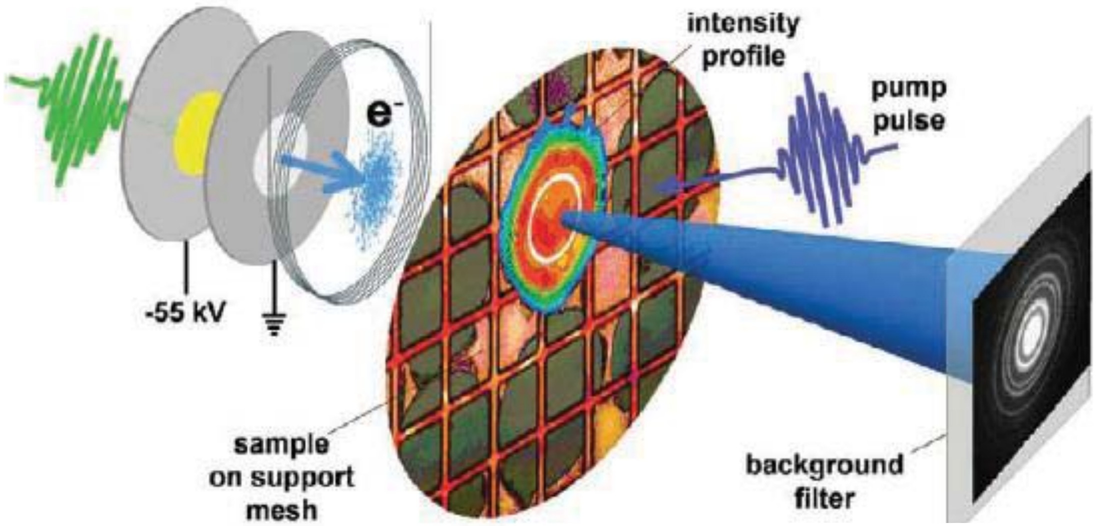

X-ray Thomson scattering (n, T)
Constant entropy curves
100.0 eV
10.0 eV
1.0 eV
0.1 eV
Temperature
Aluminum
Adiabatic expansion
pump intensity
Debye temp.
Melting Temp.
2ϕ
0.1
1.0
10.0
Density (g/cc)
pump laser
melting
boiling
ionizing
expanding
cooling
droplet formation
Electron diffraction(melting, disordering)
Photoelectron spectroscopy (energy state of electrons)

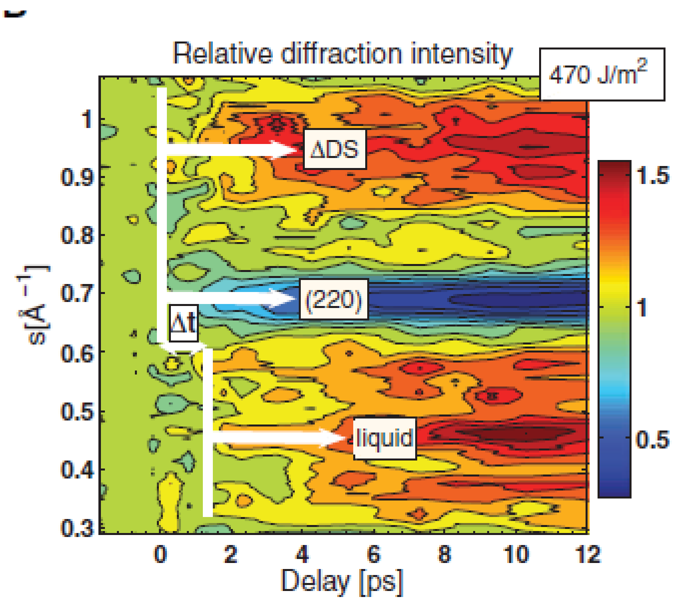
New measurement method

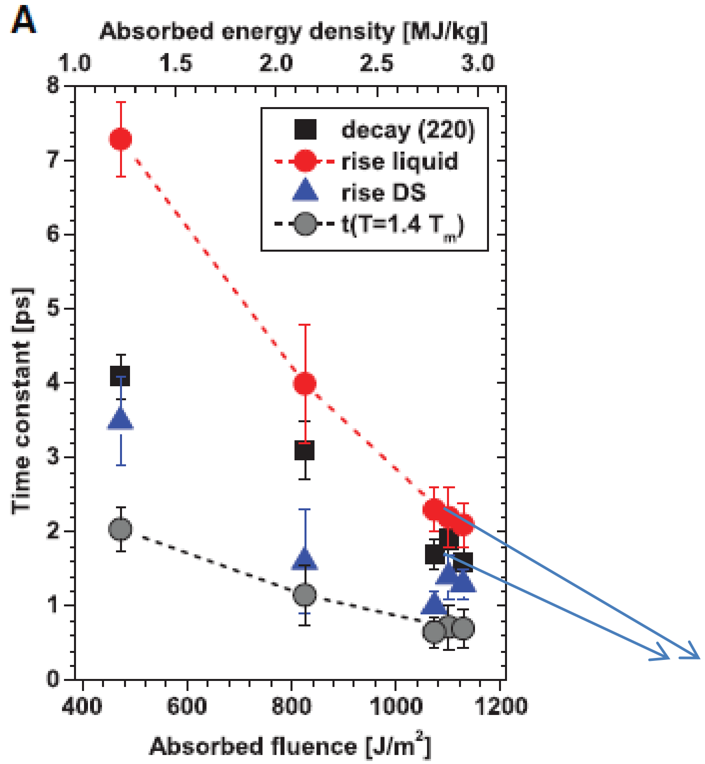
- Electron diffraction experiment
- Angle-resolved photoemission spectroscopy
- X ray scattering and transmission experiment

Electron diffraction experiment

Ralph Ernstorfer, SCIENCE, 2009 VOL 323

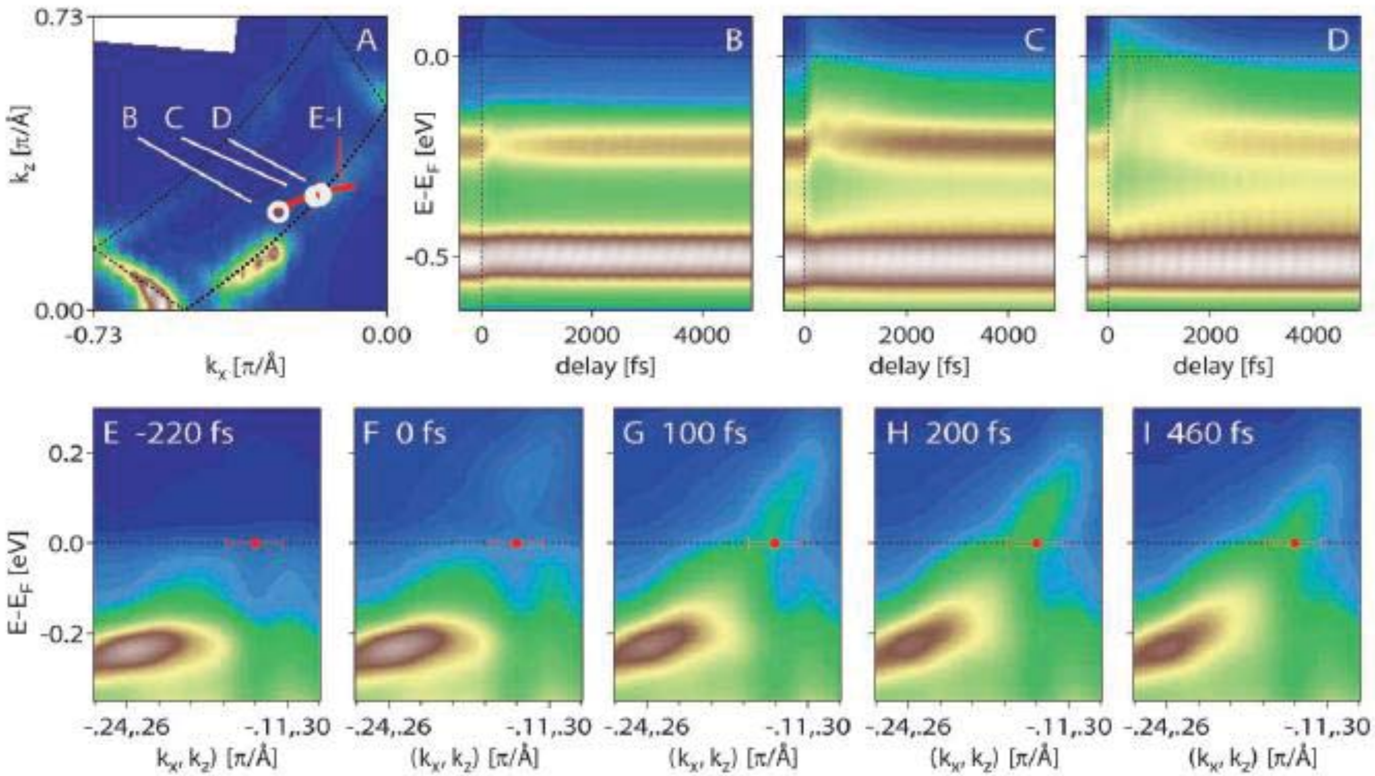


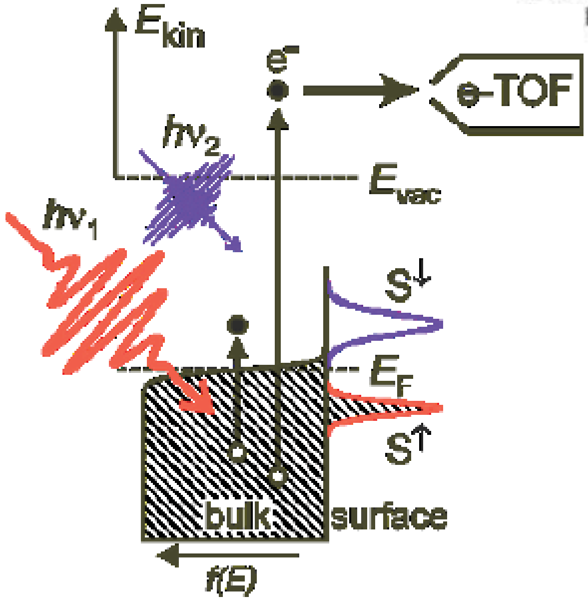




Angle-resolved photoemission spectroscopy

Fig. 3. (**A**) Detail of the FS plot in Fig. 1A′ with indicated positions (white circles) of time-resolved data shown in (**B**) to (**D**) for fixed *k* as a function of time delay. Indicated cut position (red line) of photoelectron intensity is shown as a function of energy, and position [(**E**) to (**I**)] for a momentum scan is shown as a function of time delays. All data were collected at 100 K and $F = 2$ mJ/cm^2. k_F is marked in (E) to (I) (red dot). Error bars indicate the distance to the neighboring sample points, which is a good estimate for the error of k_F.



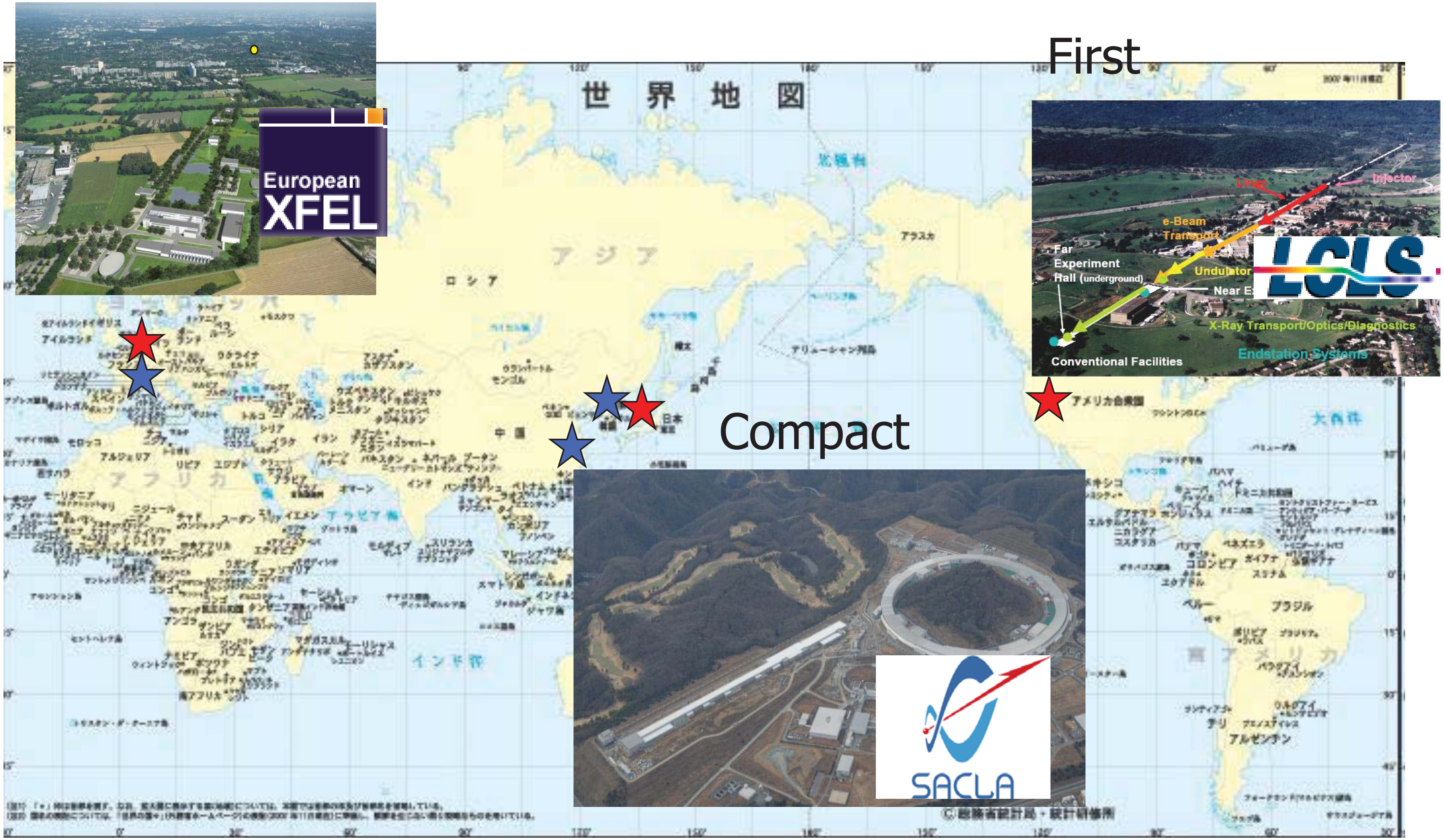


F. Schmitt, *et al., Science* **321**, 1649 (2008);

Martin Wolf, European XFEL SCS Workshop, PSI, 2 - 4 June 2009

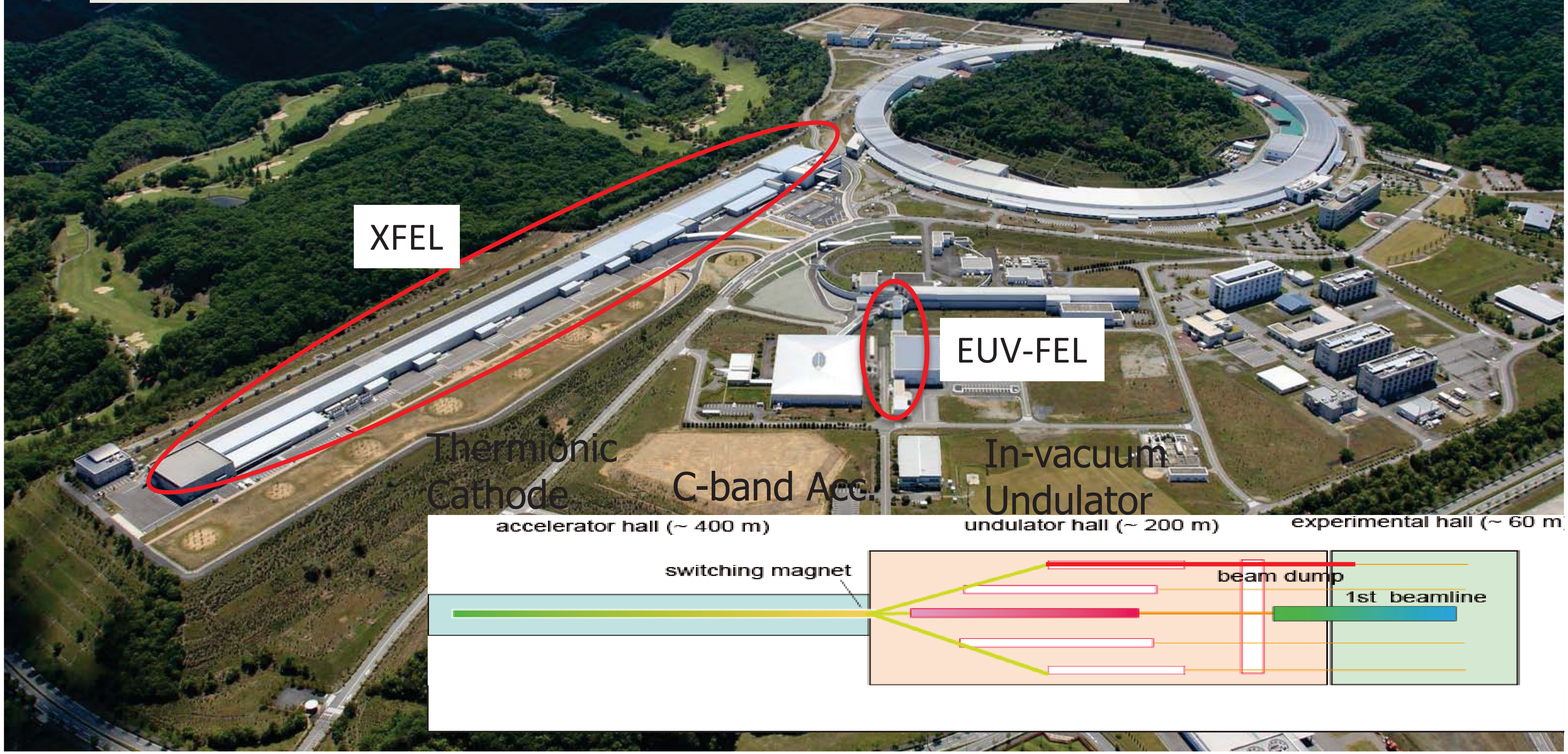
XFEL sources in the world

High rep rate

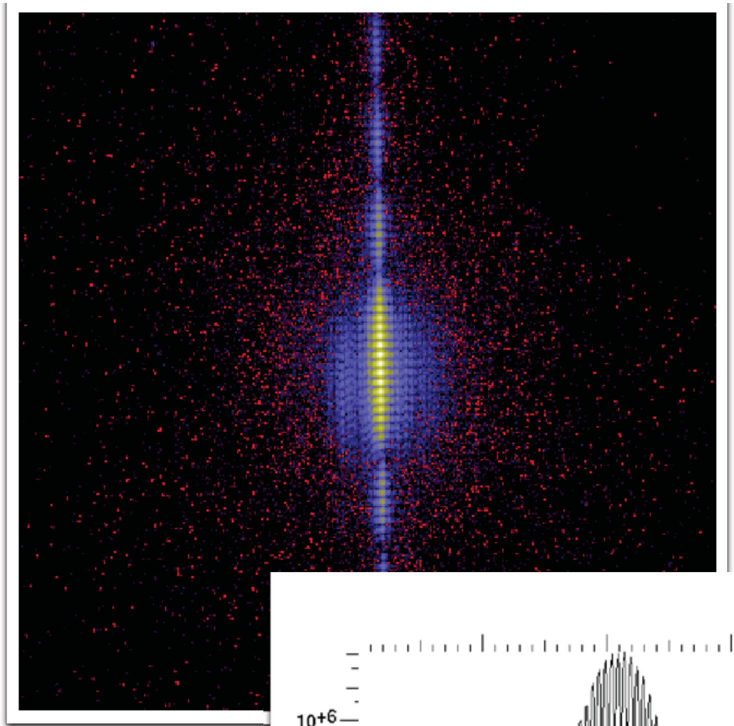


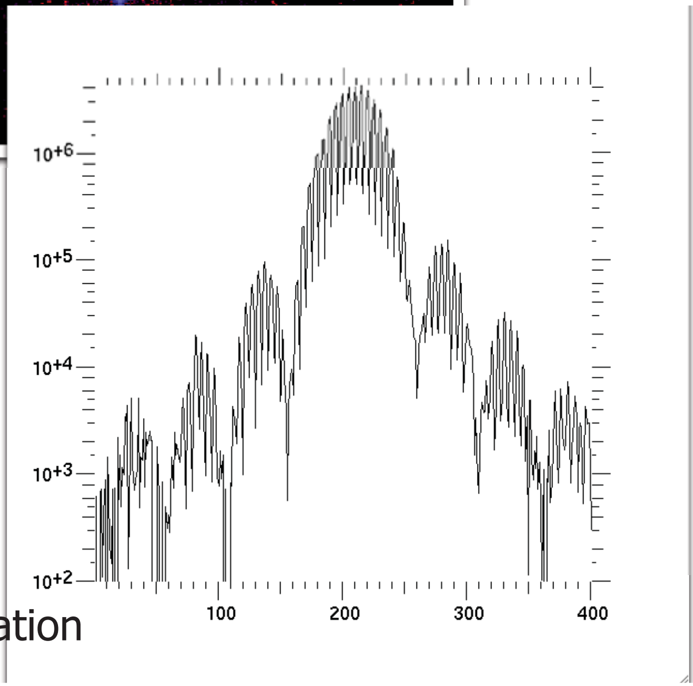
SACLA & EUV FEL @SPring-8

Compact XFEL
Construction: FY2006~2010
User Operation: FY2011~ **(7 March 2012)**



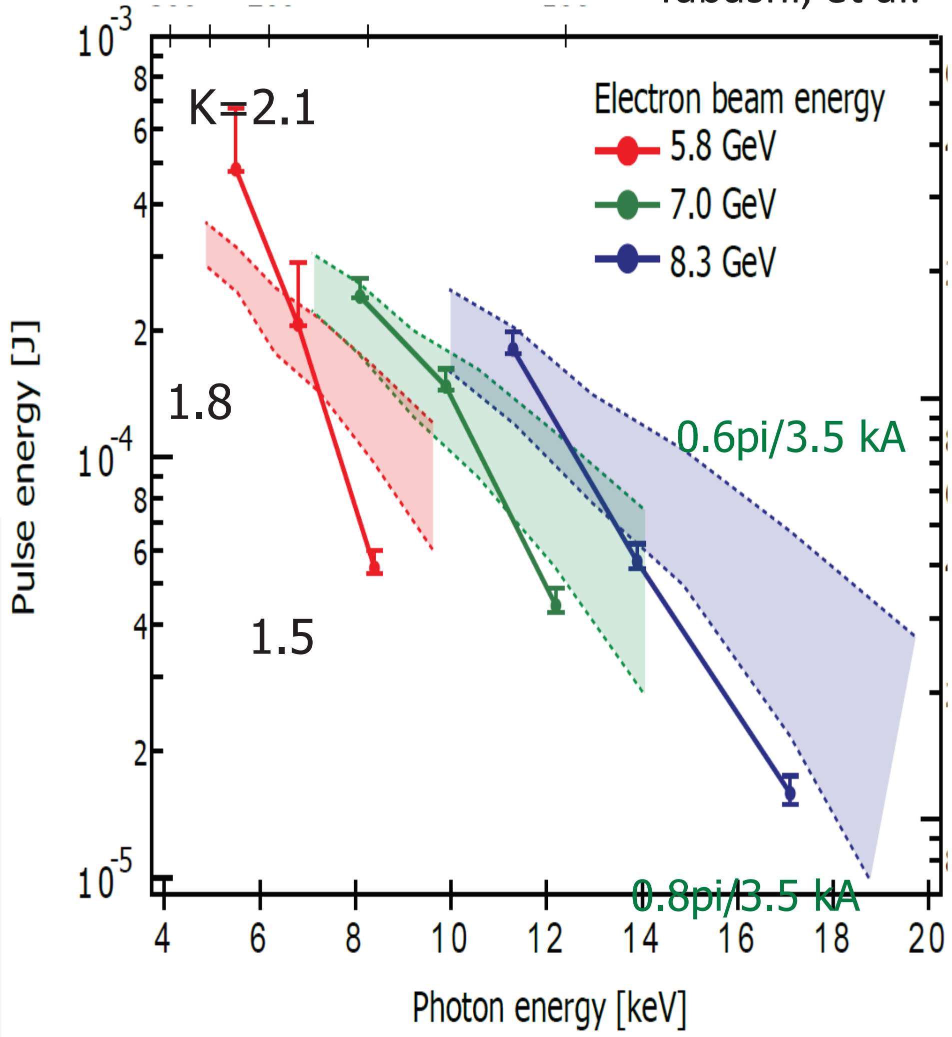
Coherence & Wavelength & Pulse energy





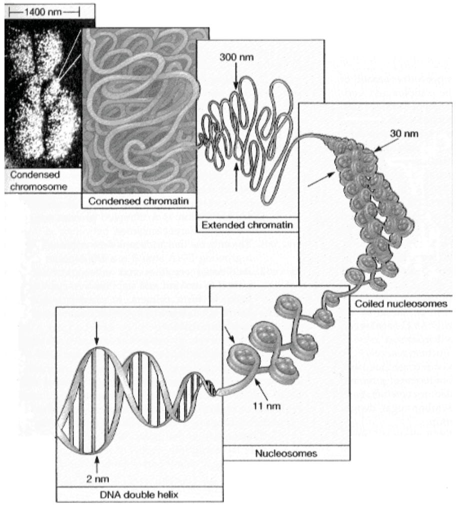
Song et al
5 um width
50 um separation

Yabashi, et al.

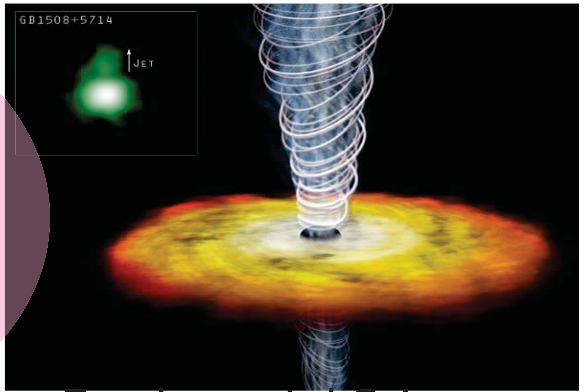


under review

XFEL explores new worlds of science



Brilliance (X10^9)

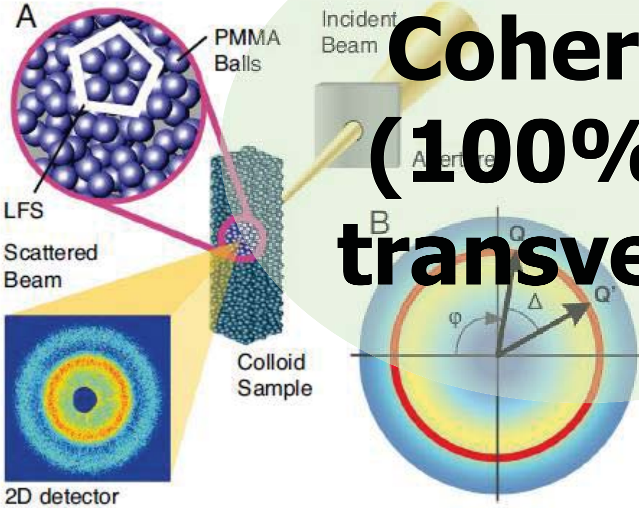


Fundamental Science: Create Extreme State

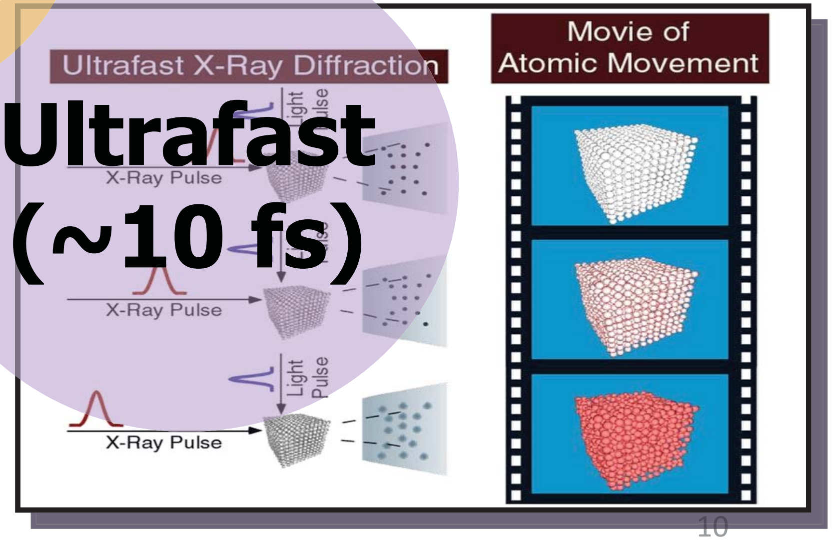
XFEL

Biology & Medicine: Investigate non-crystalline materials

Environmental & Energy Science: Probe ultrafast reactions



Coherent (100% in transverse)



Ultrafast (~10 fs)

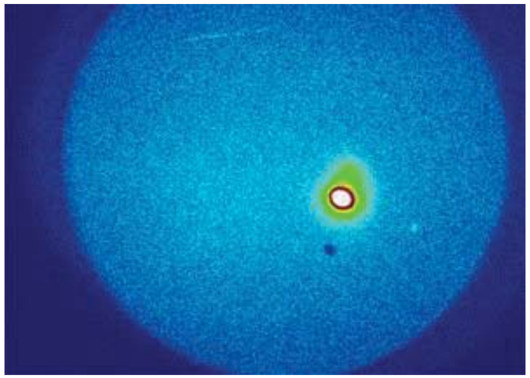
How intense of X-ray?

- X-ray Free electron laser(from 2011) I~10^{21}W/cm^2

  5~20keV, ~mJ, ~10fs, focus diameter ~50nm(min. 7nm), 60Hz

- EUV Free electron laser (since 2006) I~10^{15}W/cm^2

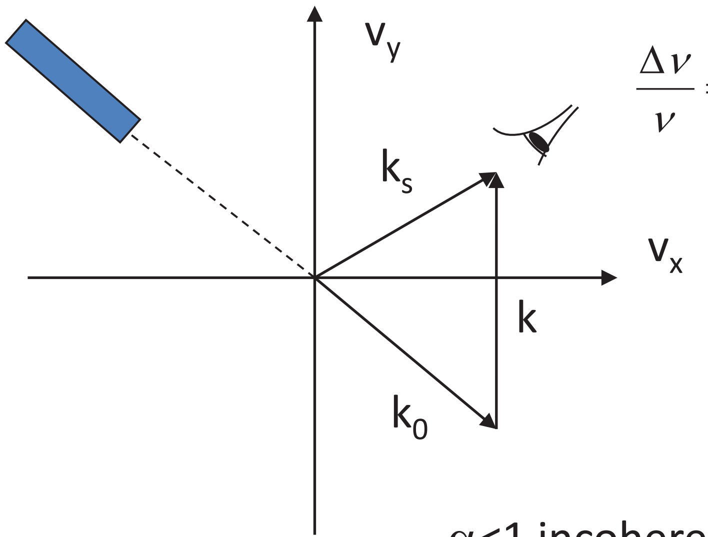
  45~170nm, ~20μJ, ~60fs, focus diameter ~6μm, 30Hz



Diagnostics for Warm dense matter with X-ray

Thomson Scattering

$$\alpha = \frac{\lambda_{Laser}}{4\pi\lambda_D \sin(\theta/2)} = 1/k_{Laser}\lambda_D \sin(\theta/2) = \frac{\lambda_{Laser}}{4\pi \sin(\theta/2)}\left(\frac{4\pi ne^2}{kT_e}\right)^{1/2}$$



$$\frac{\Delta\nu}{\nu} = \frac{v_y}{c} 2\sin\frac{\theta}{2}$$

collective or incoherent?

α<1 incoherent (independent electron
=> electron velocity distribution function)

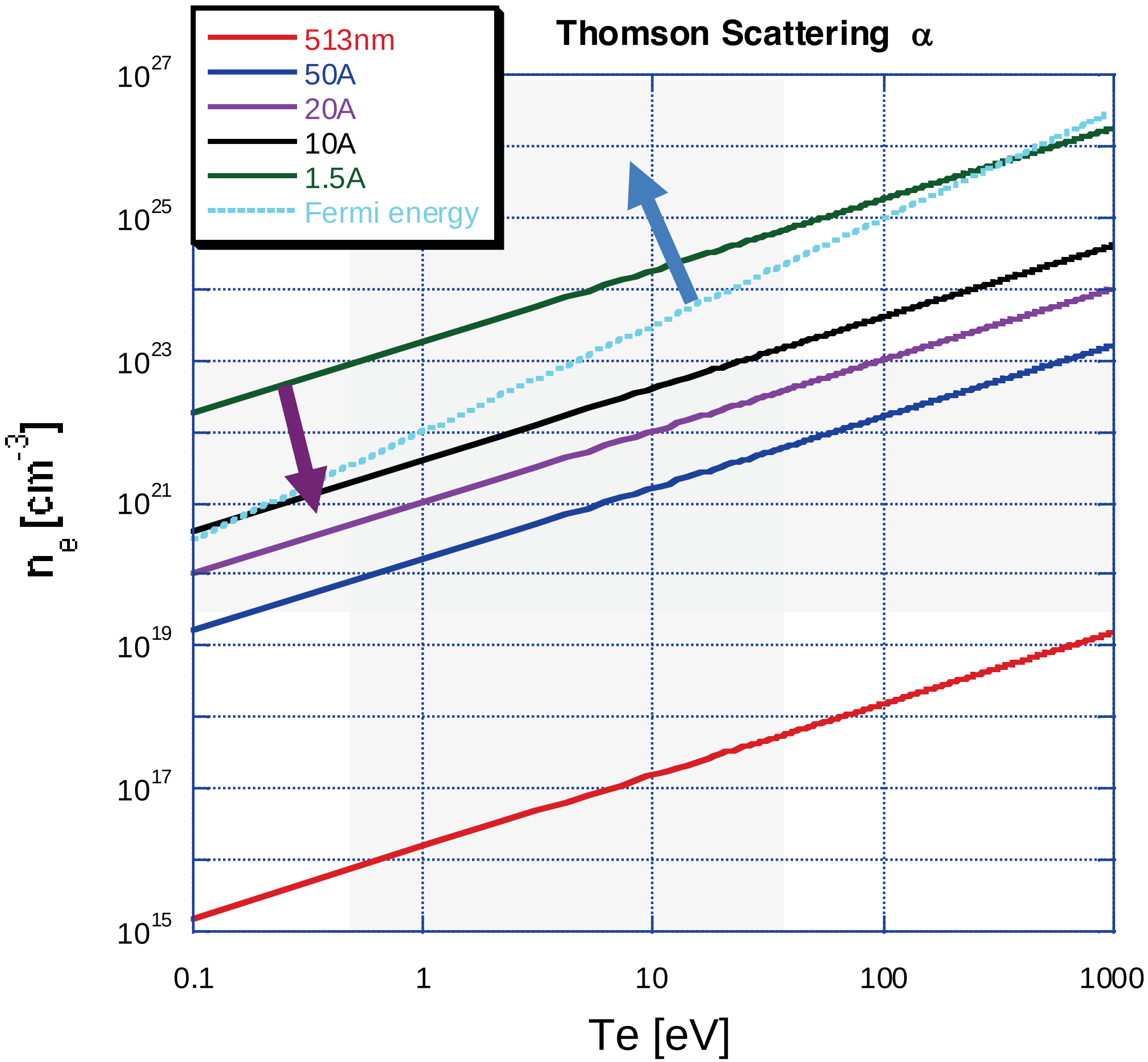
α>1 collective (ion acoustic wave, electron plasma wave)

dispersion relation: $\omega_0^2 = \omega_{pe}^2 + 3(kT_e/m)k^2$

spectral width ~ ion Doppler width

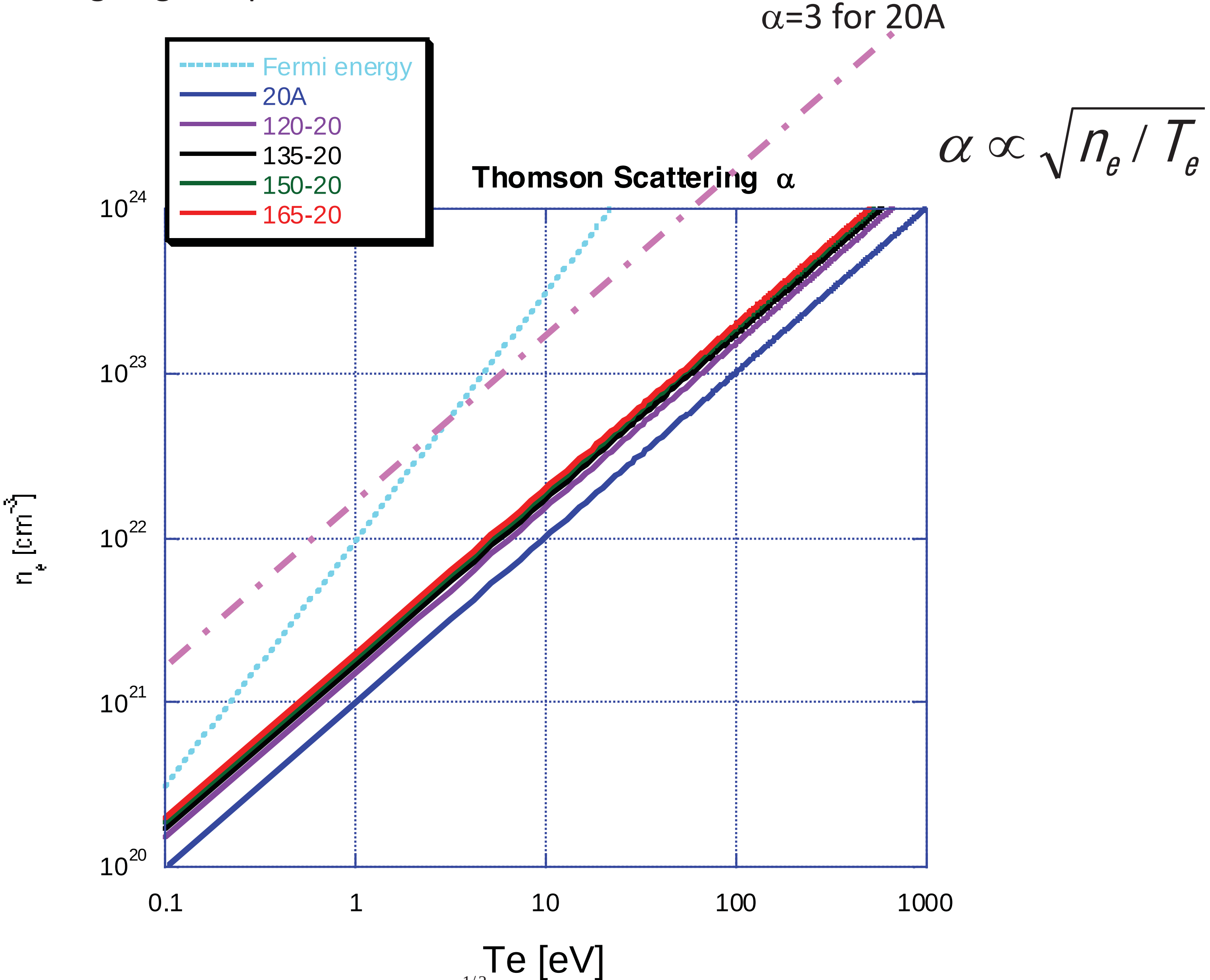
At α~1 , we can decide both of temperature and density.

α=1 line

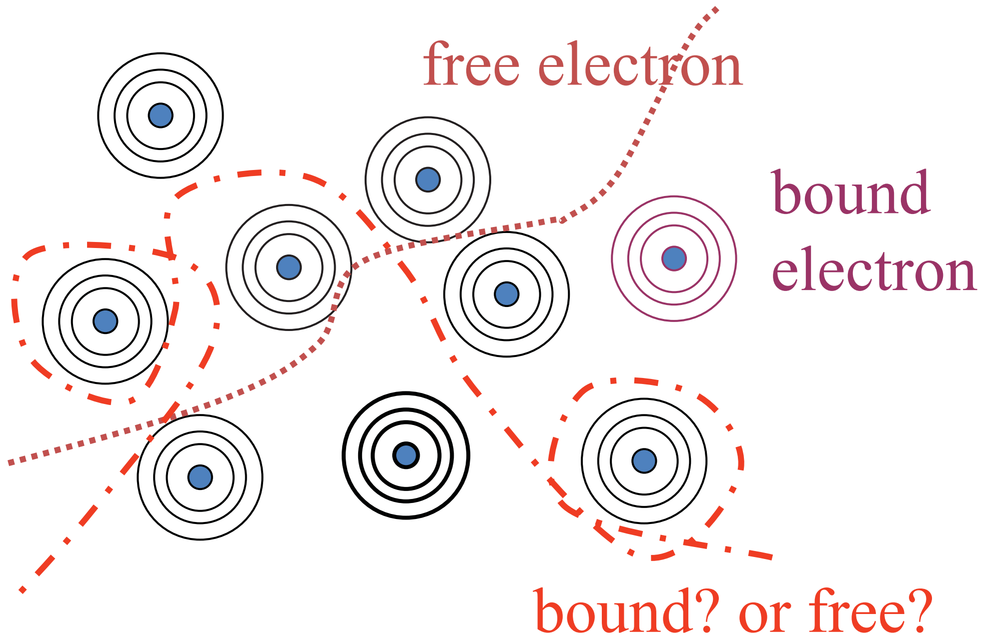


Thomson Scattering α
513nm
50A
20A
10A
1.5A
Fermi energy
10^27
10^25
10^23
10^21
10^19
10^17
10^15
n_e [cm^-3]
0.1
1
10
100
1000
Te [eV]

Scattering angle dependence



$$\alpha = \frac{\lambda_{Laser}}{4\pi\lambda_D \sin(\theta/2)} = 1/\,k_{Laser}\lambda_D \sin(\theta/2) = \frac{\lambda_{Laser}}{4\pi \sin(\theta/2)}\left(\frac{4\pi n e^2}{kT_e}\right)^{1/2}$$



Scattering cross section

density correlations of electrons <= ion motion

free electron scattering

inelastic scattering with bound electrons

$$S(k,\omega)=\left| f_I(k)+q(k)\right|^2 S_{ii}(k,\omega)+Z_f S^0_{ee}(k,\omega)+Z_c\int \tilde{S}_{ce}(k,\omega-\omega')S_s(k,\omega')d\omega'$$

ion form factor

screening cloud of free and valence electrons

ion-ion density correlation function

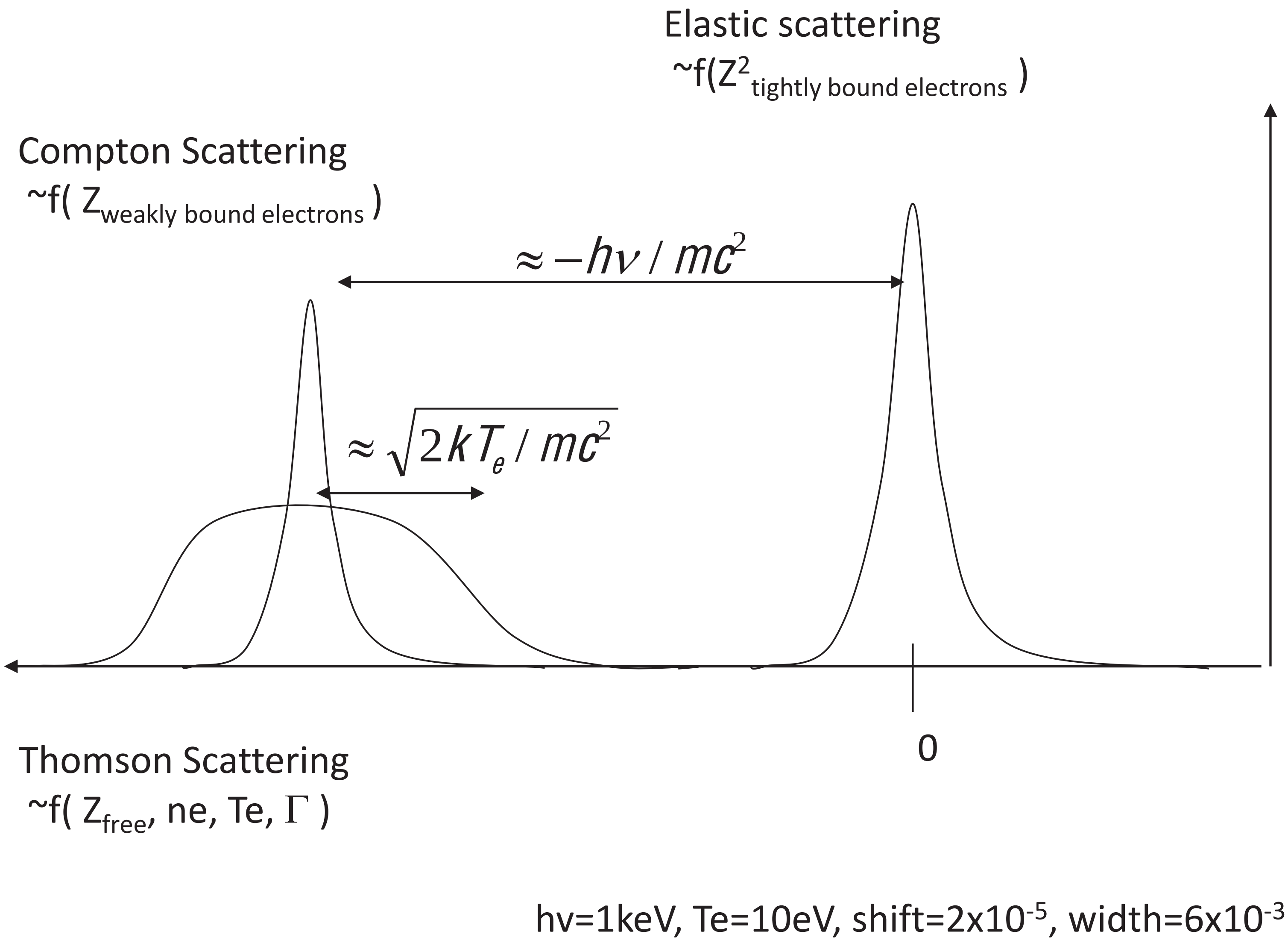
charge for free electron

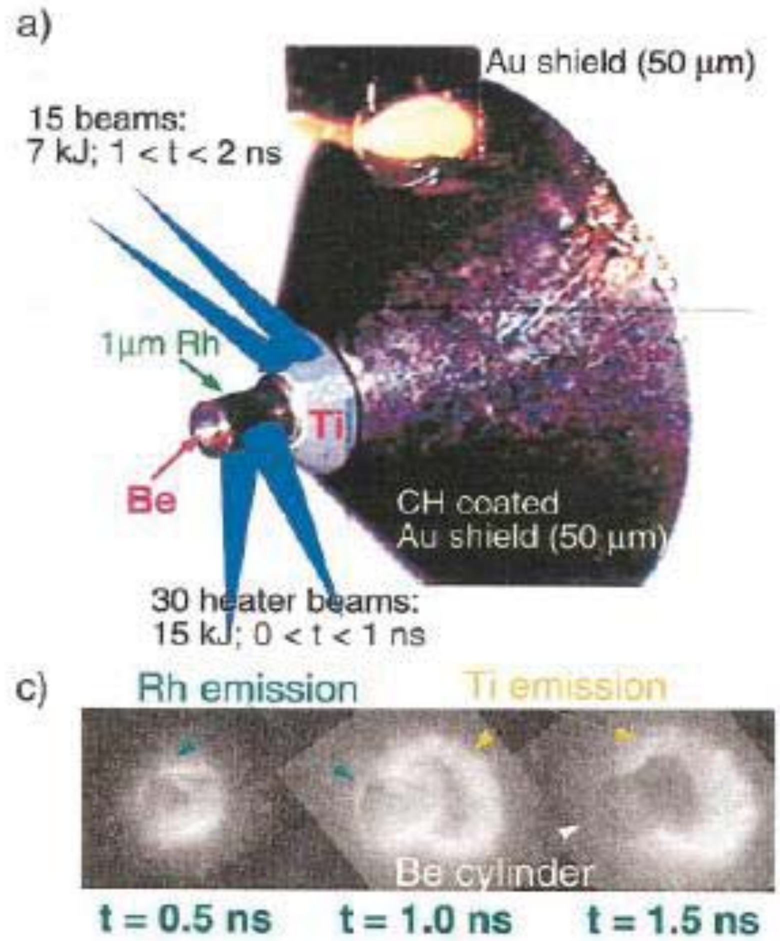
high frequency part of e-e correlation function

charge for bound electron

bound-free transition

self-motion of ions


Elastic scattering
~f(Z²tightly bound electrons)
Compton Scattering
~f(Zweakly bound electrons)
$\approx -h\nu / mc^2$
$\approx \sqrt{2kT_e / mc^2}$
0
Thomson Scattering
~f(Zfree, ne, Te, Γ)
hv=1keV, Te=10eV, shift=2x10-5, width=6x10-3



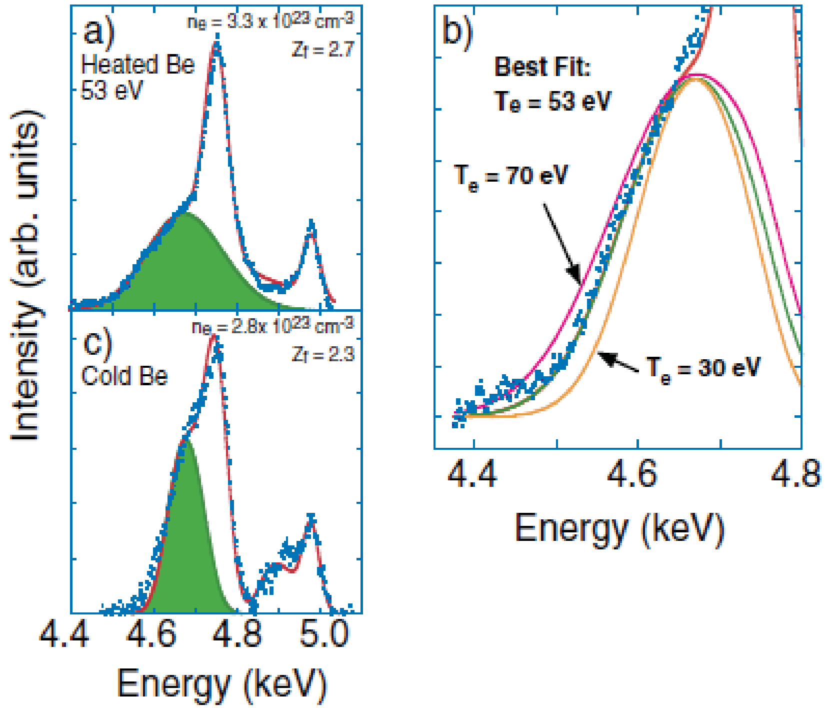


FIG. 3 (color). (a) Experimental x-ray scattering data (blue dots) from the heated Be plasma with a theoretical fit yielding $T_e = 53$ eV and $n_e = 3.3 \times 10^{23}$ cm^{-3}. (b) Red wing of the scattering spectrum together with the best fit and calculated spectra for $T_e = 30$ eV and $T_e = 70$ eV indicating that the electron temperature is determined with 10%–20% accuracy. (c) Experimental x-ray scattering data (blue dots) from the cold Be indicating $T_e \approx 2$ eV and $n_e = 2.8 \times 10^{23}$ cm^{-3}. The green shaded area corresponds to the Compton down-shifted feature as obtained from the fit.

S. H. Glenzer,PRL, Vol.90, No.17, 175002 (2003)

PHYSICS OF PLASMAS VOLUME 11, NUMBER 5 MAY 2004

Electronic structure measurements of dense plasmasa.

G. Gregori, et al.,

4.75keV Ti He-α (dλ/λ<0.005)

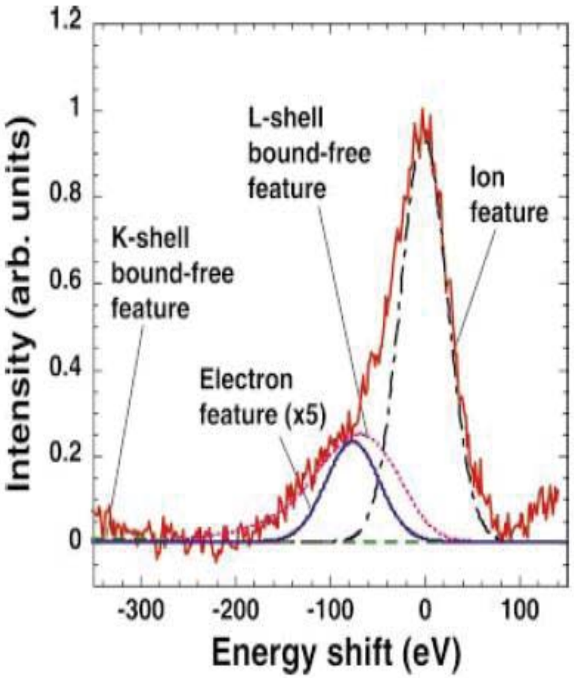


FIG. 6. (Color) Spectrum of the unheated foam with separated contributions from each different scattering mechanism. Convolution with instrument response is added each terms. The probe radiation is the Ti He−α line at 4.75 keV, and the scattered x rays are collected at ~130°±5° scattering angle with best fit parameters T_e<5 eV and Z_f=0.26. The ionization energy for isolated neutral carbon is E_B^0=11 eV for L-shell electrons and E_B^0=286 eV for K-shell electrons.

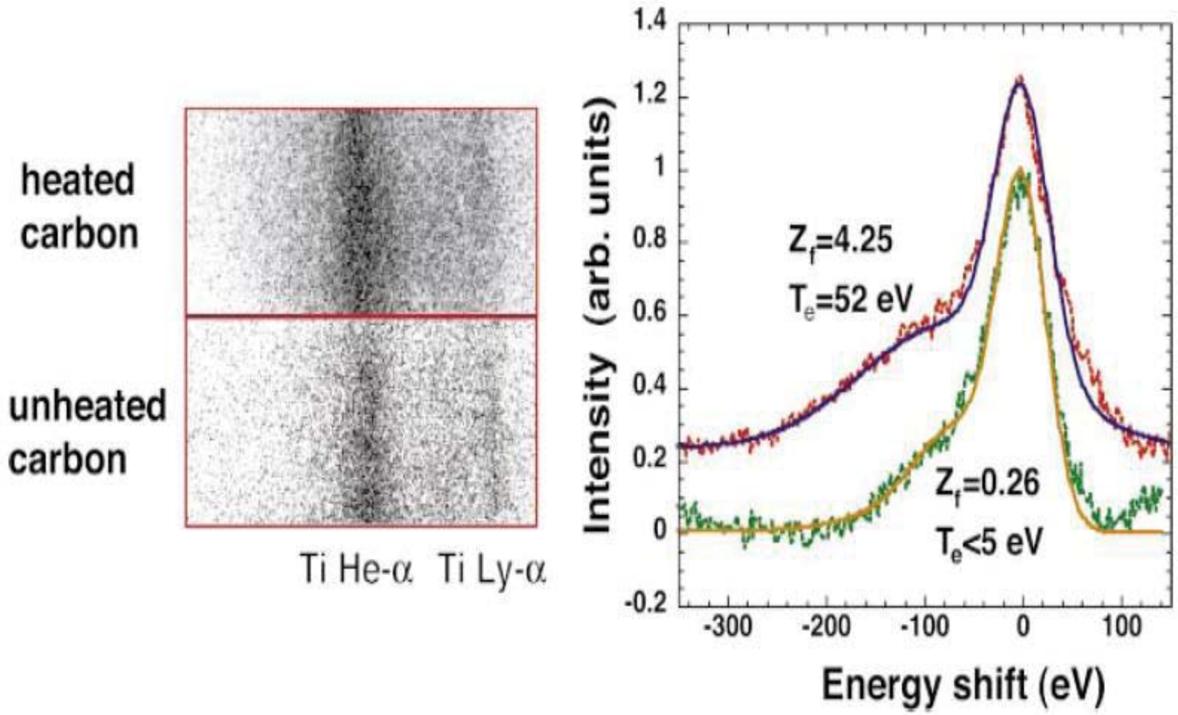


FIG. 4. (Color) Experimental x-ray scattering data from a heated carbon foam (0.72 g/cm^3) and a cold (unheated) carbon foam. The raw data, as measured by the detector are shown on the left side. Lineouts and best fits are reported on the right panel. The probe radiation is the Ti He−α line at 4.75 keV, and the scattered x rays are collected at ~130°±5° scattering angle. Best fit parameters and corresponding spectra are also plotted in the figure. For the high temperature foam, α=0.17, T_F=10.4 eV, and Γ=0.2; while for the cold foam α=0.13, T_F=1.6 eV, and Γ=0.9.

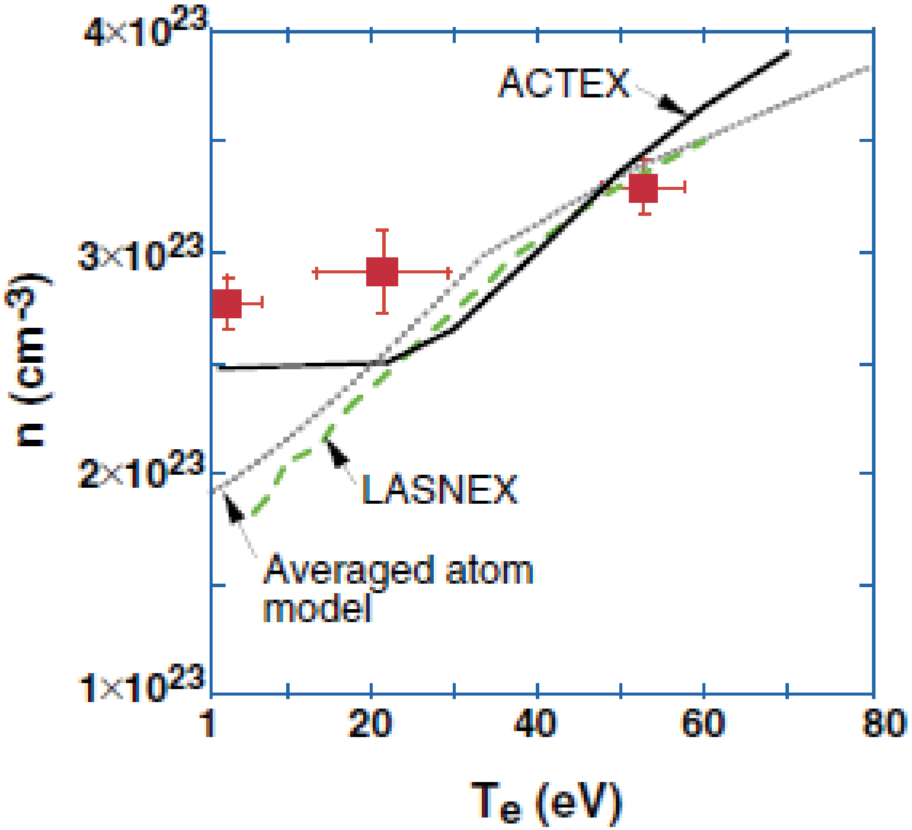
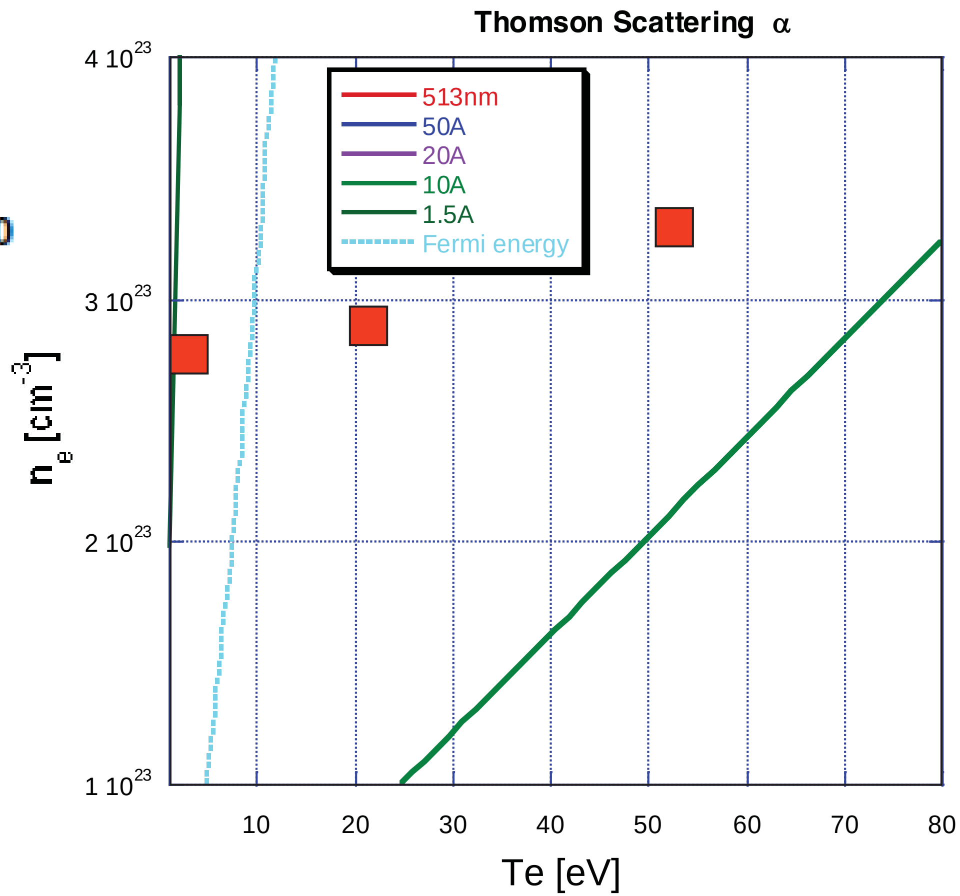


FIG. 4 (color). Density-temperature phase diagram along with the results of the x-ray scattering measurements and simulation using the ACTEX model [18], an averaged atom model [19], and radiation-hydrodynamic modeling [20]. The data and the ACTEX model include the free plus weakly bound (conduction) electrons. The averaged atom model and LASNEX only include free (ionized) electrons.

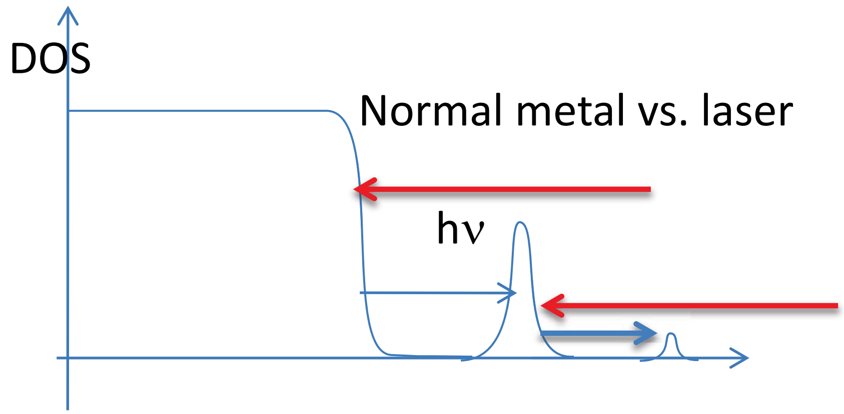
λ=2.6A

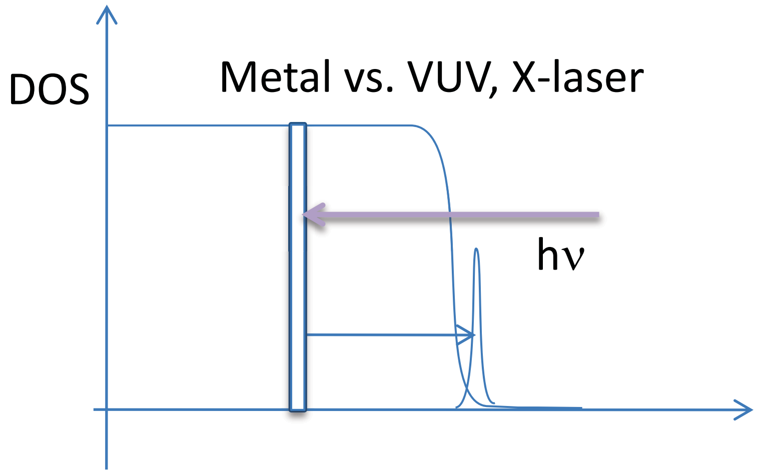


Creation of new states of matter

What different in interaction physics with XFEL?

absorption



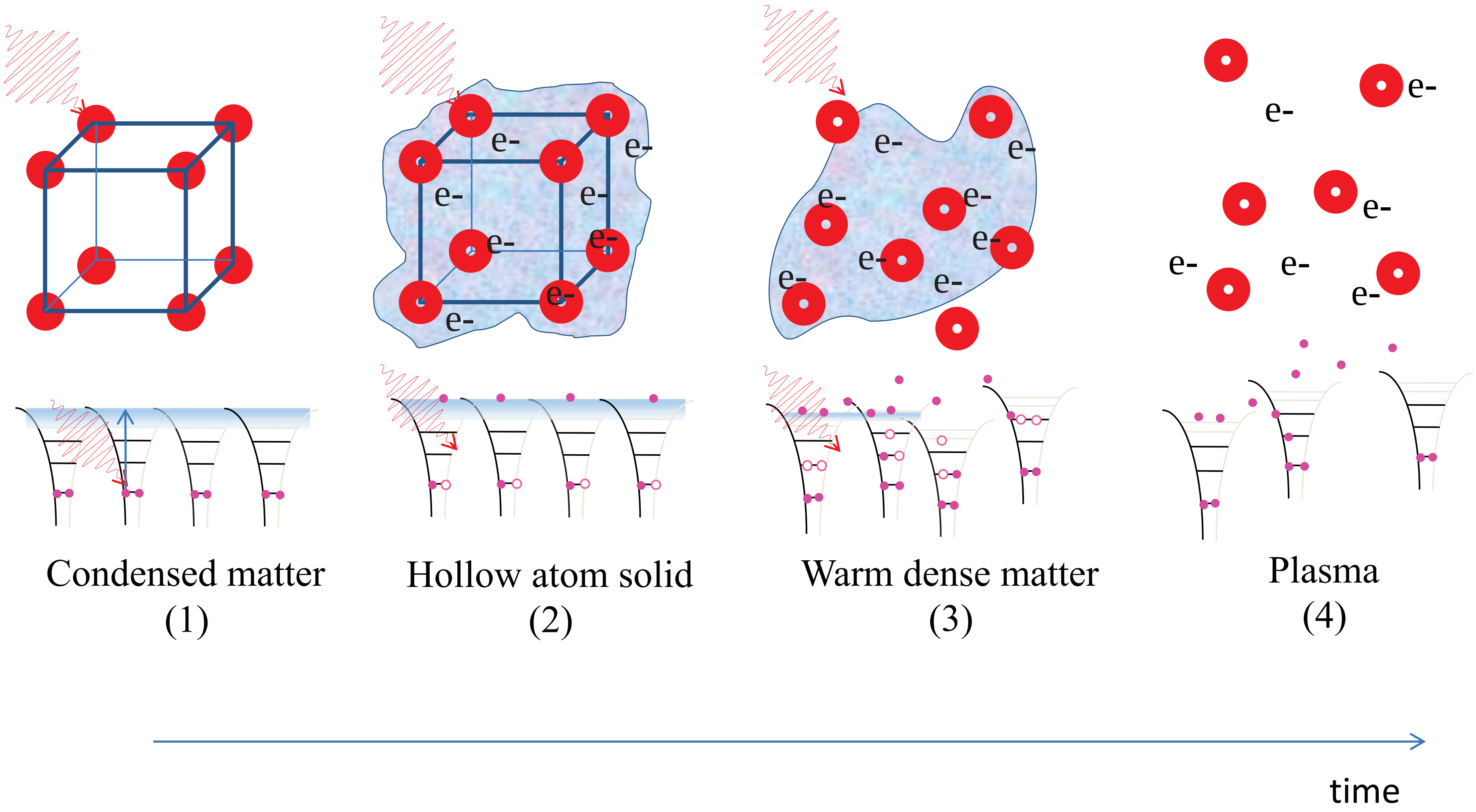


$$n_{e_{solid}} < n_c \; for \; \mathrm{EUV, Xray}$$

There is No effect of preplasma even in high intensity laser interaction.

It is easy to penetrate into solid density.

Material condition



High energy density matter

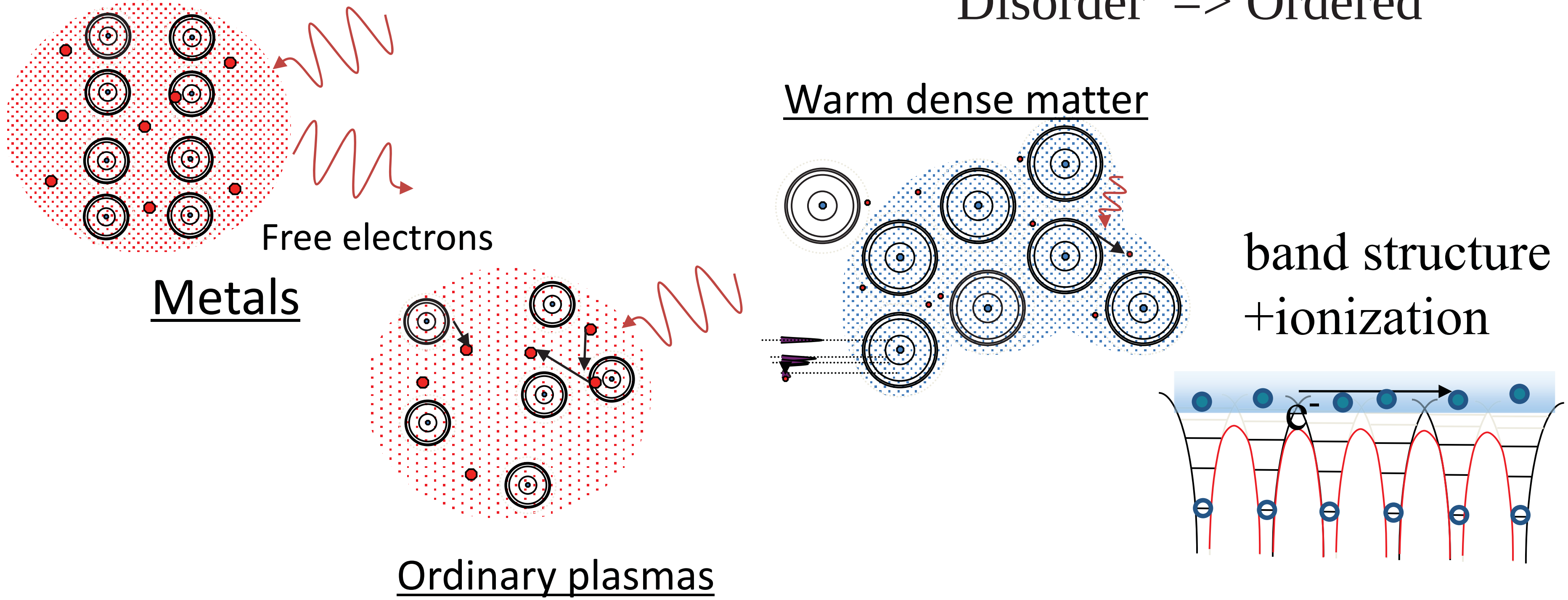
Xray & EUV laser interaction experiments

Ion excitation Energy

$$F[\rho, T] = E_{cold}[\rho] + F_{elec}[\rho, T] + F_{ion}[\rho, T] + E_{excitation}$$

EOS internal energy | Cold curve | Electron-Thermal | Ion-Thermal

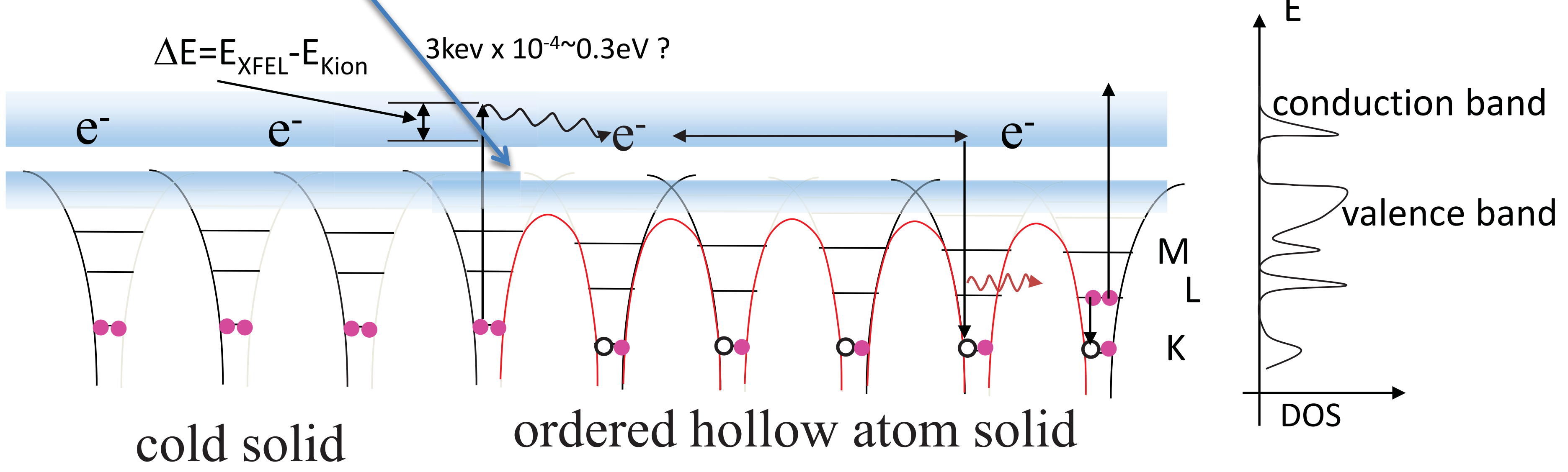
Disorder => Ordered



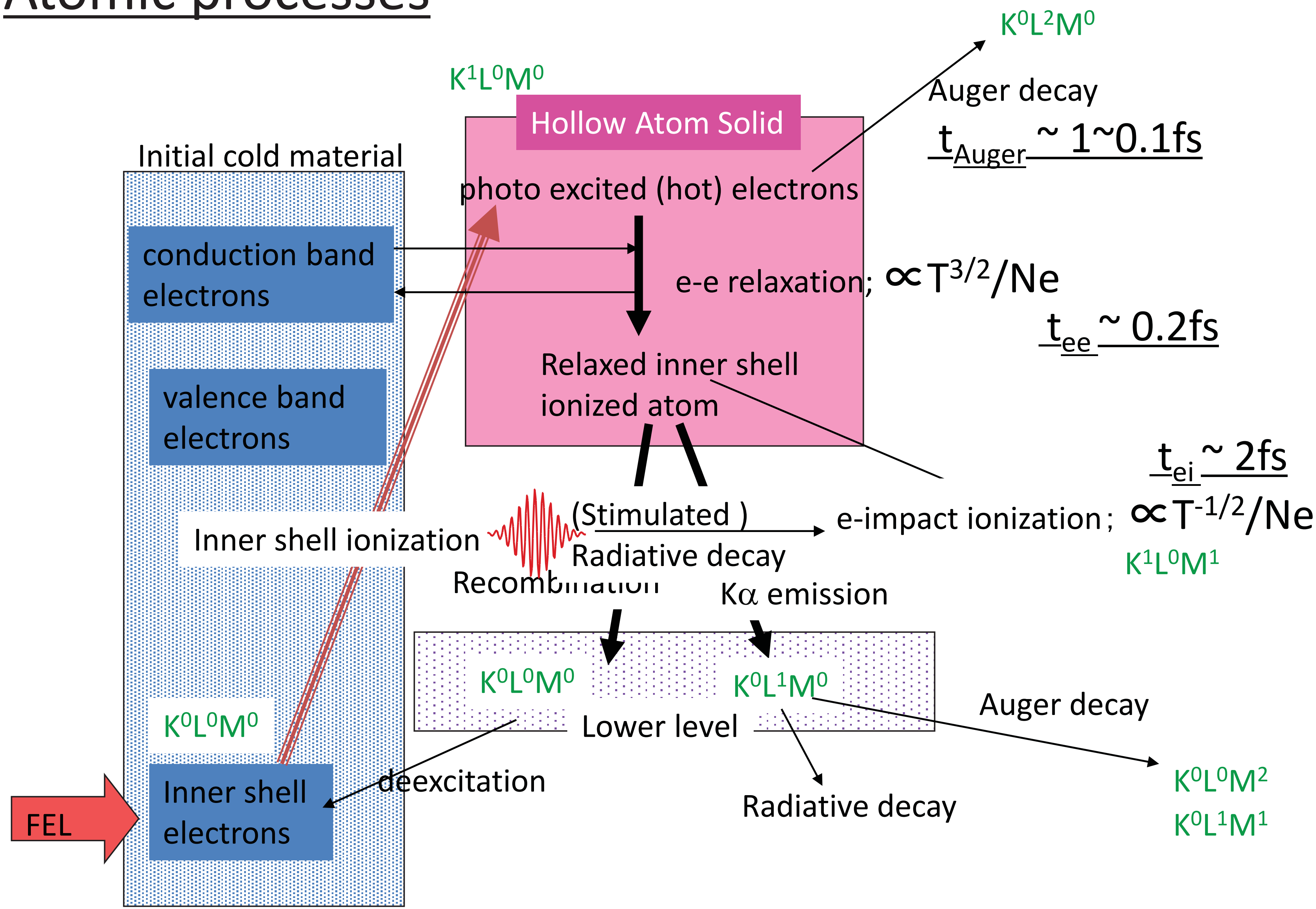
Well-tuned X-ray and EUV laser photon

If $t_{pulse} < t_{disassemble}$, we create ordered solid with inner shell excited ions.

We can expect large optical parameter change in X-ray.



Atomic processes



What different in interaction physics with XFEL? (cont.)

Speed of excitation can be higher than relaxation rate of atomic process in solid.

$$\frac{dN}{dt} = \frac{\alpha I}{h\nu} \quad \Rightarrow \quad \tau_{excitation} = \frac{N}{dN/dt} = \frac{N_{solid}}{\alpha I} h\nu$$

EUV interaction has big advantage because large α and smaller $h\nu$.

(We can sustain inner shell hole under radiation.)

α at Ti K edge ~ 3350cm^{-1} at 5keV => τ <1fs for I>10^{18}W/cm^2

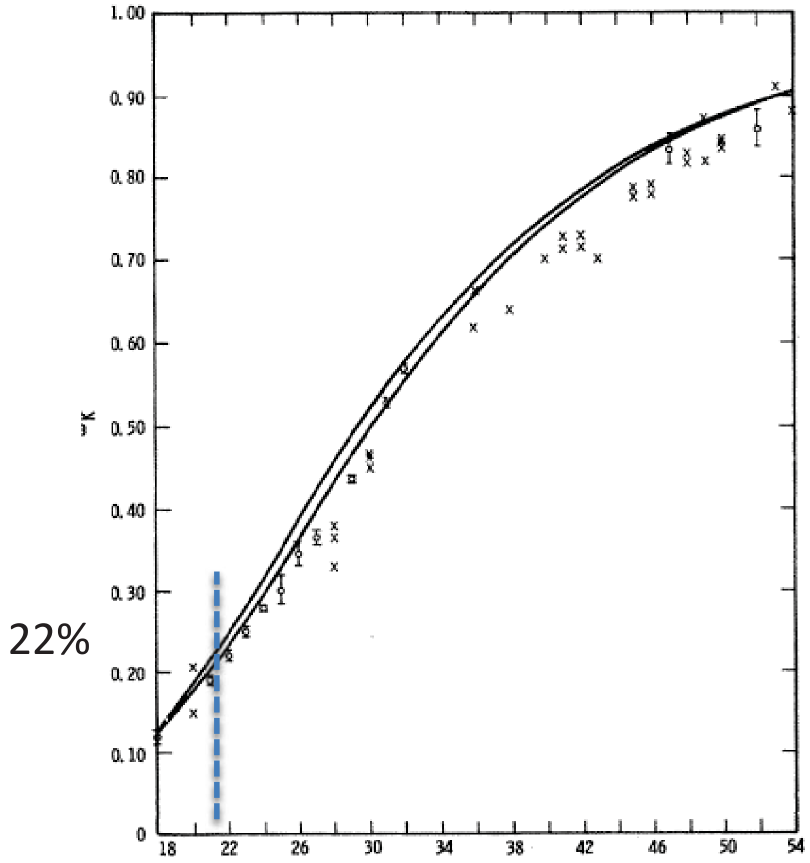


FIG. 1. *K*-shell fluorescence yield versus *Z*. The upper curve is the uncorrected; the lower the corrected calculations. The data points with error bars are from Refs. 5–11, and the crosses from Ref. 12.

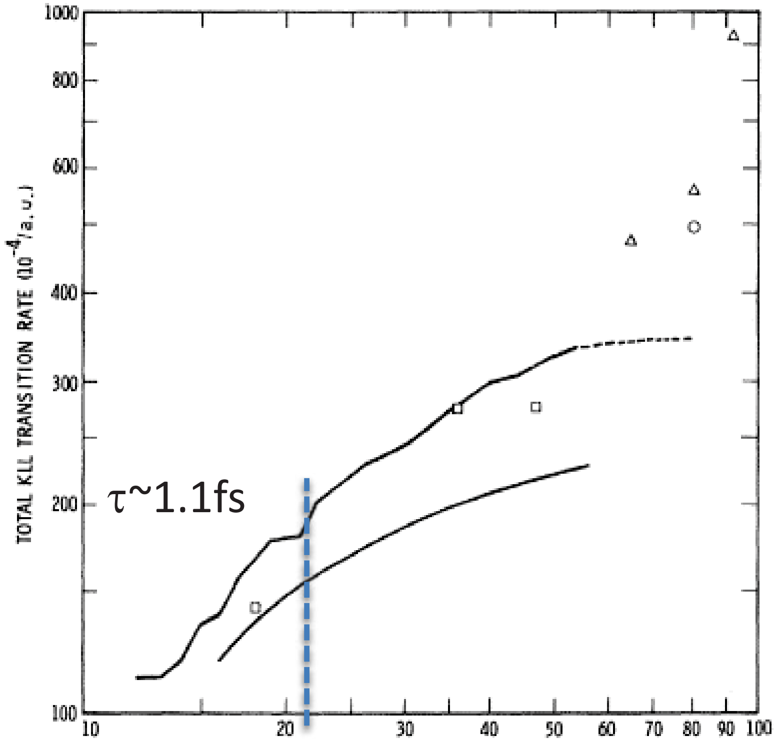


FIG. 3. Total *KLL* Auger rate versus *Z* in 10^{-4}/a.u. (1 a.u. = 2.42×10^{-17} sec). The upper solid curve is from our calculations; the dashed portion was obtained for *Z* = 60, 65, 70, and 80 for which we did *KLL* calculations only. The lower solid curve is from Ref. 19; the squares from Ref. 36; the circle from Ref. 20; and the triangles from Ref. 21.

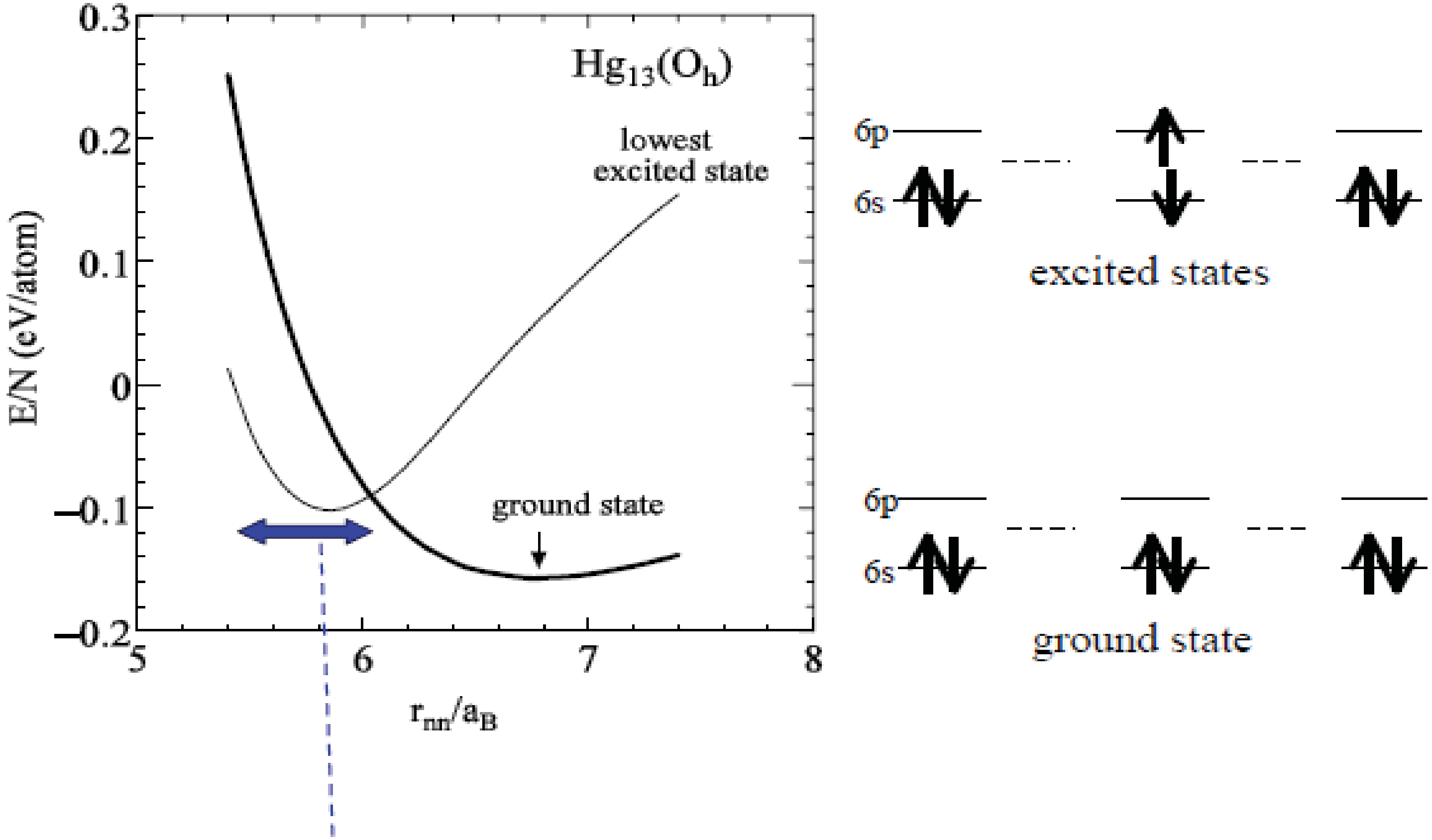
E. J. McGuire, Phys. Rev. A 2, 273–278 (1970)

α at Ti K edge ~ 3350cm^{-1}

$$\frac{dN}{dt} = \frac{\alpha I}{h\nu}$$

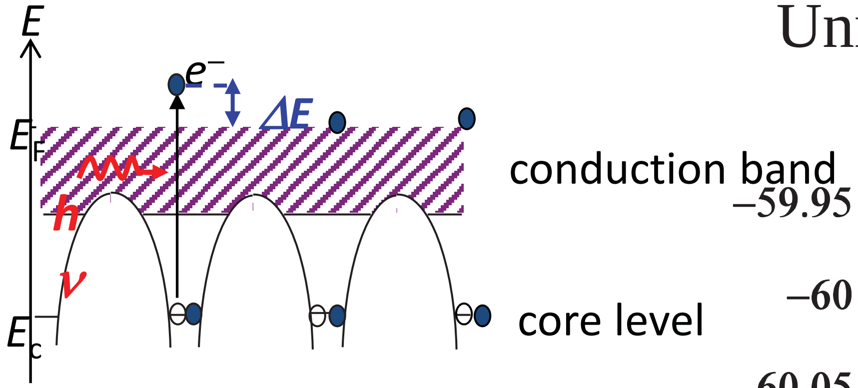
If I = 10^{18}W/cm^2, (dN/dt/N)$^{-1}$ ~ τ_{Auger}.

potential energy curve of Hg_{13} (cuboctahedron)

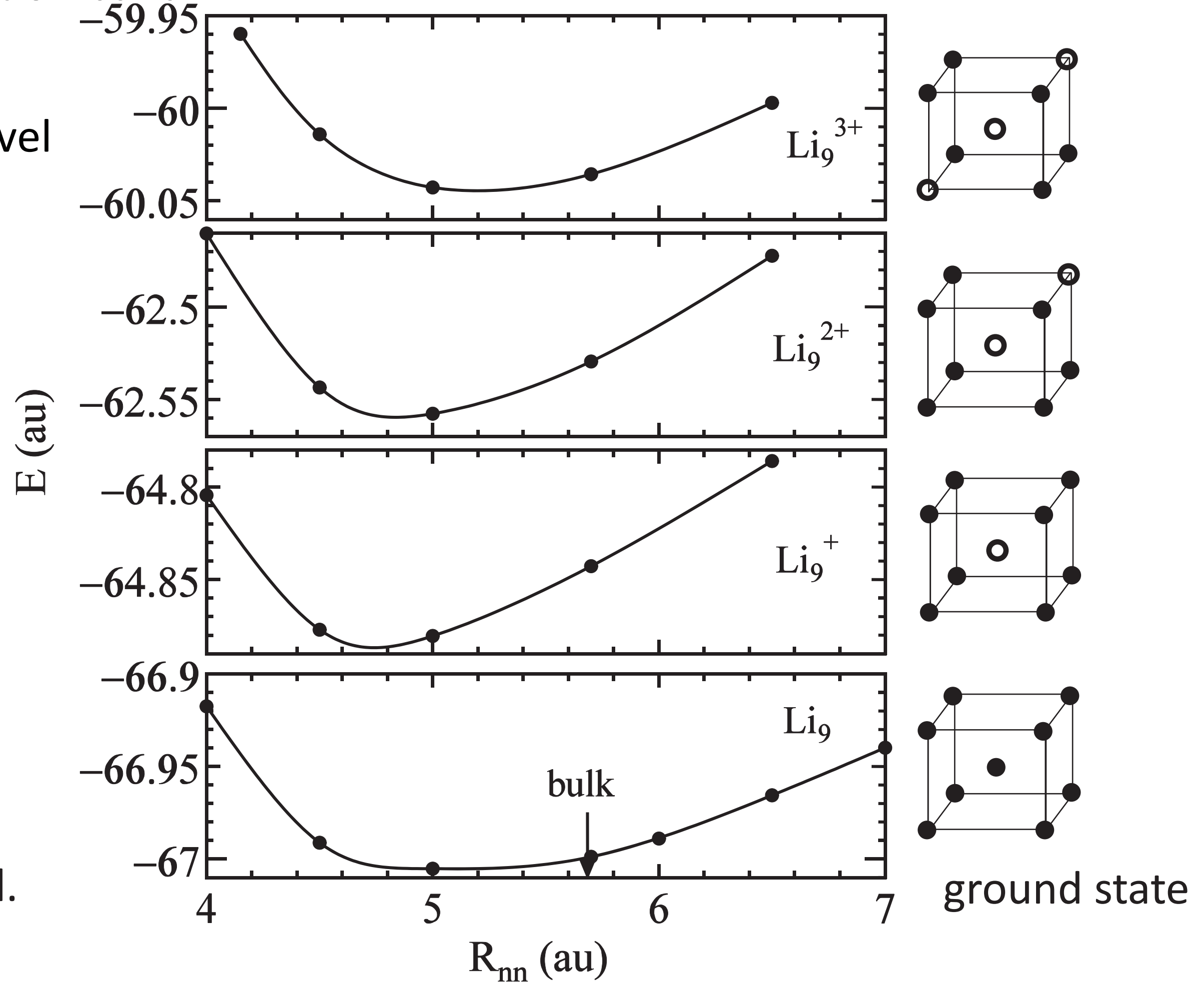


"excitonic ground state" for $r_{nn} < 6.0$ *a.u*
--- *large admixture of p-state*

Potential energy curves for Li_9^{Z+} ions



Unrestricted Hartree-Fock calculations



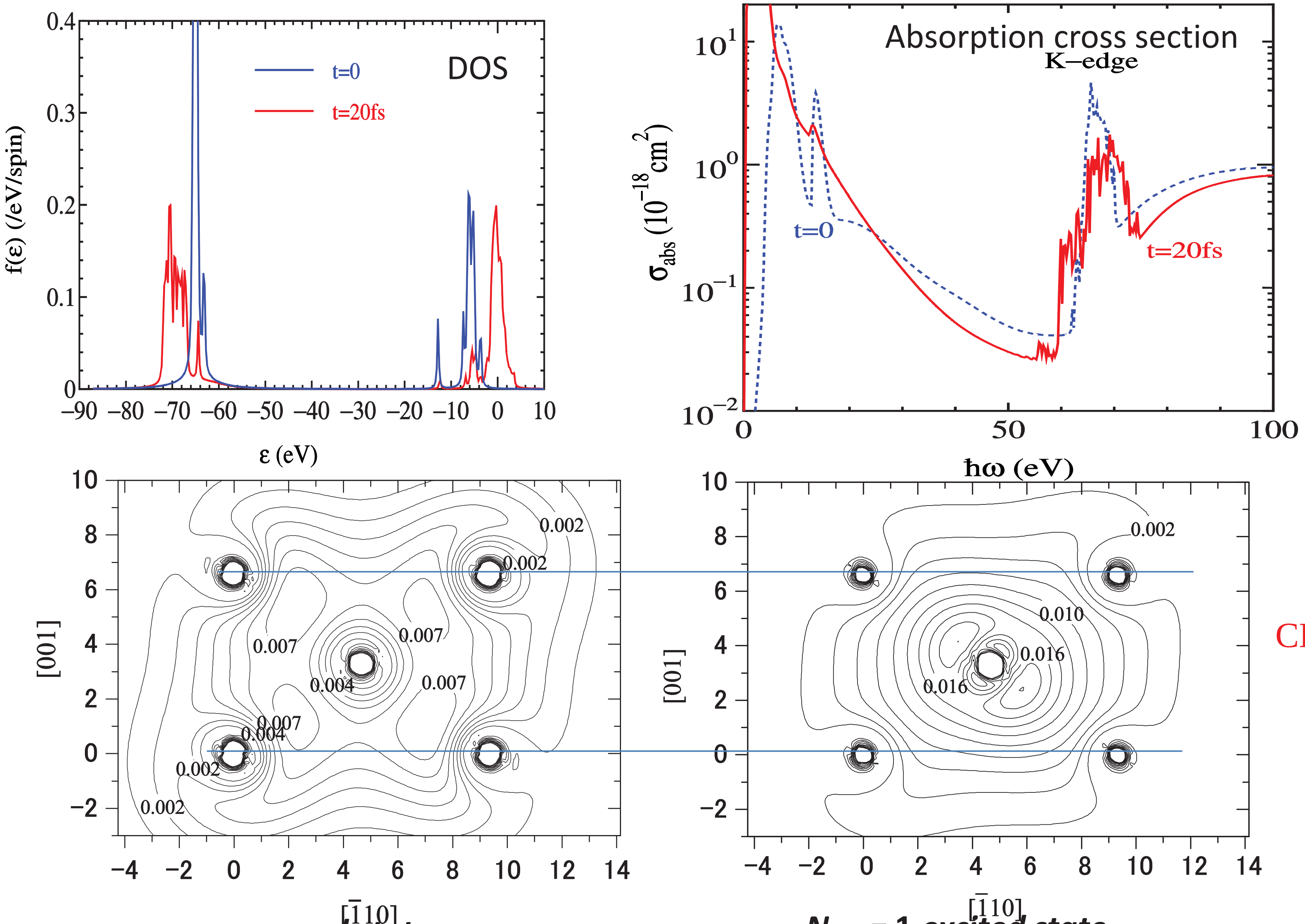
Clusters are bound
at least for $Z \leq 3$!

A key point is ionized electrons
are trapped in the conduction band.

H. Kitamura, Eur. Phys. J. D **52**, pp.147-150 (2009)

Energy state after illumination of resonant Xray

Li24 cluster calculation



ground state

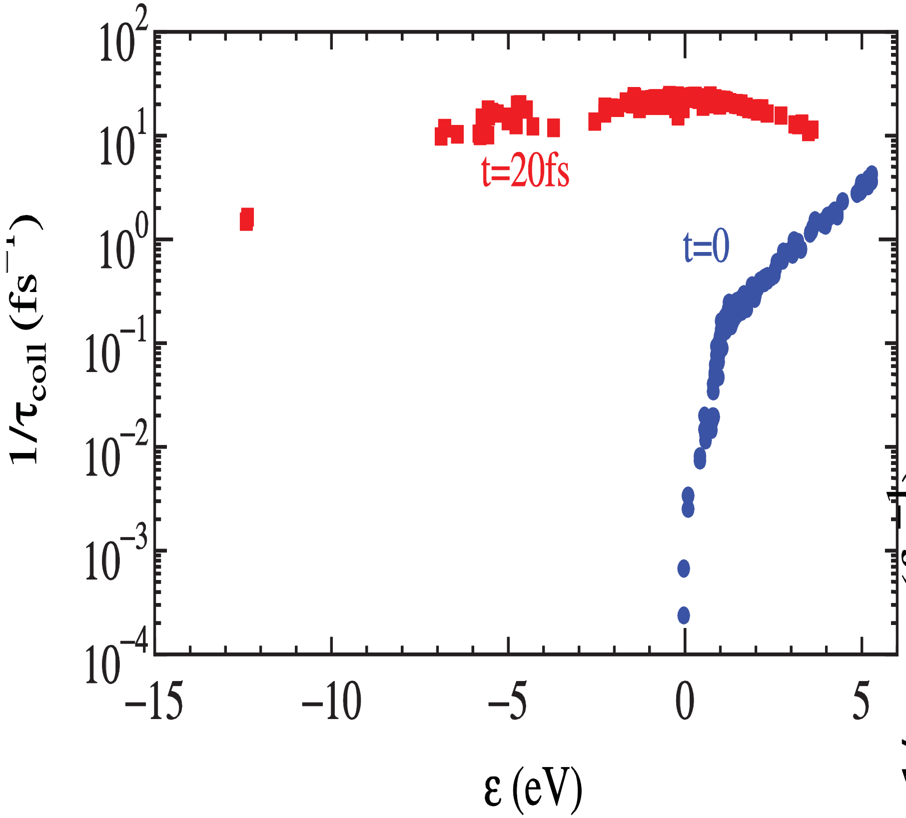
N_{exc} = 1 excited state

CHAS

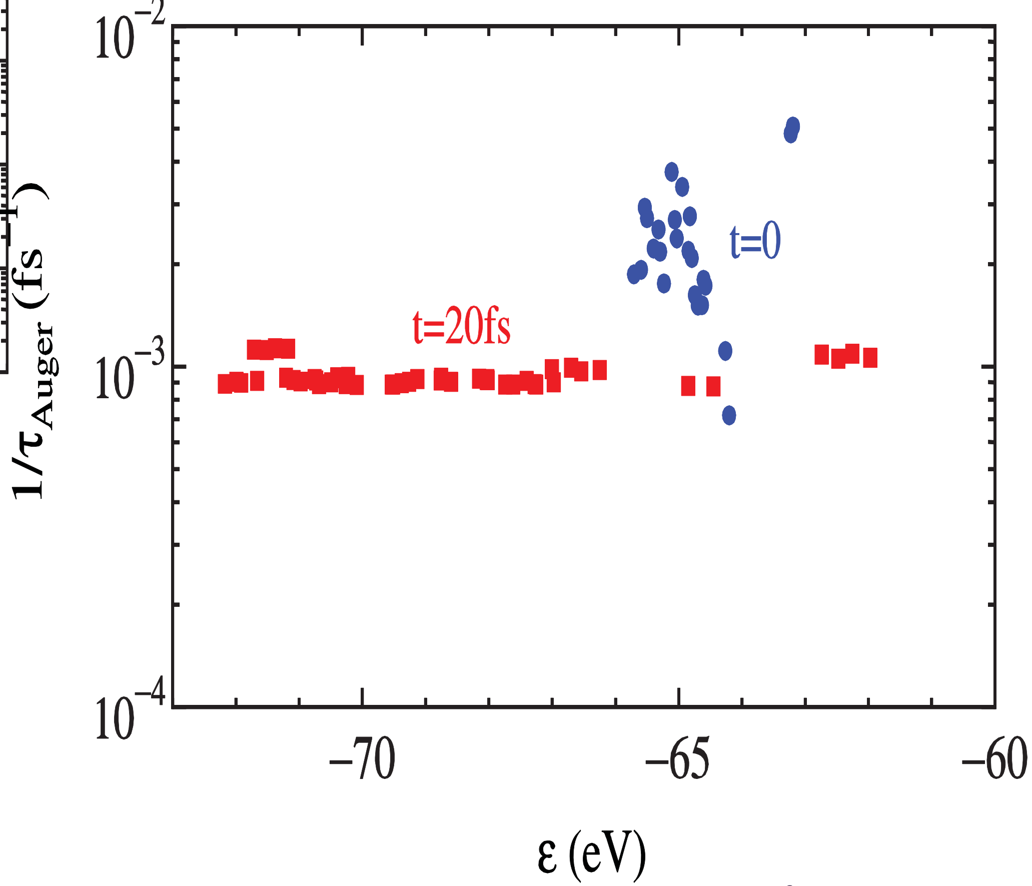
H. Kitamura, 2008

24 Li atoms cluster

Electron collision relaxation time

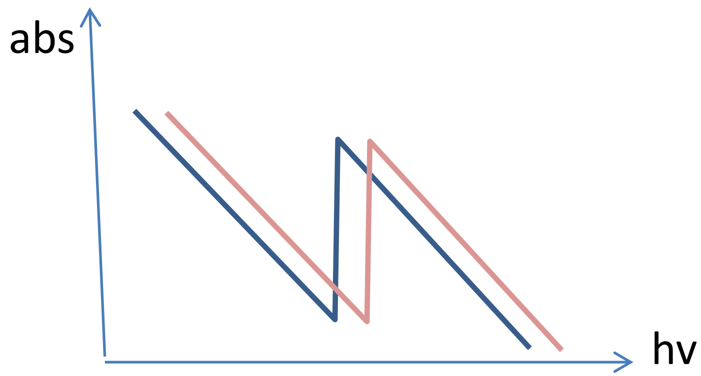


KVV Auger decay rate



H. Kitamura, 2008

K edge shift due to L vacancy



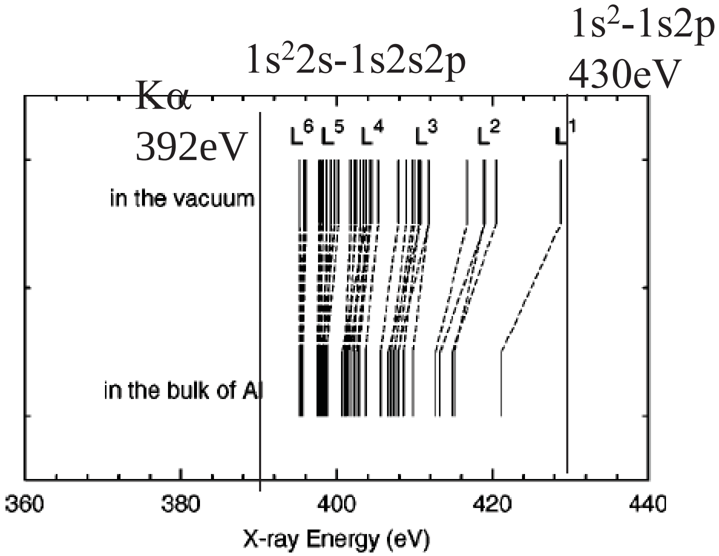


FIG. 3. The x-ray spectra emitted from N^{q+} hollow atoms and ions in the bulk of Al and in vacuum.

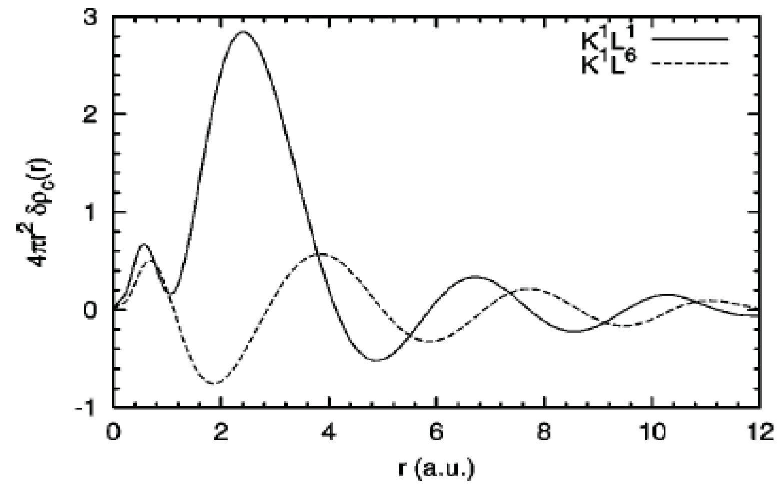


FIG. 2. Conduction electron density changes due to the perturbation of N^{q+} hollow atoms or ions in the bulk of Al.

$KLM \Rightarrow K^1LM \Rightarrow K^0L^2M$ → $K^0L^1M^2$

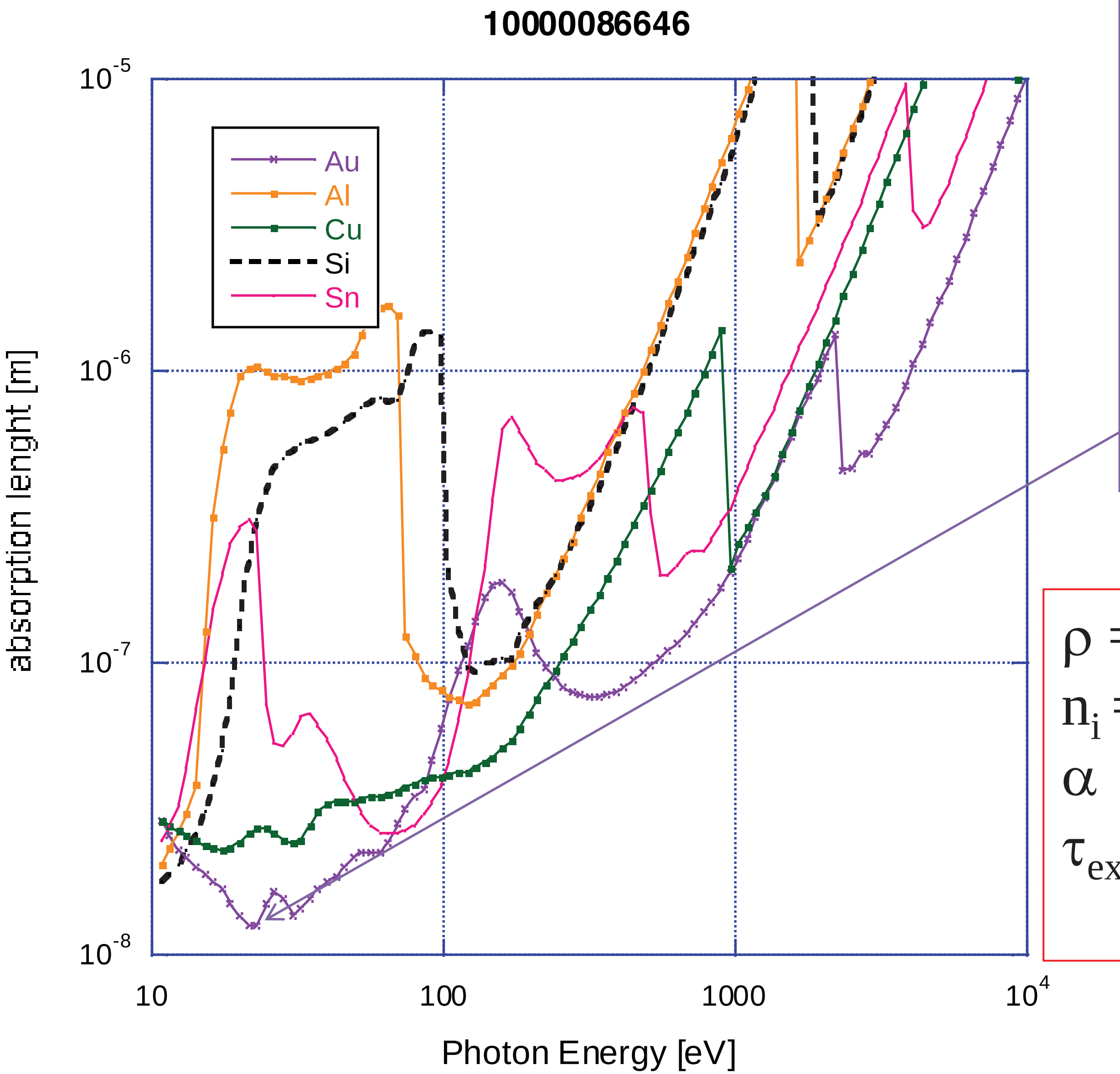
→ $K^1L^2M^0$ → $K^0L^4M^0$ → $K^0L^3M^2$

→ $K^2L^0M^0$

X. M. Tong, Phys. Rev. A 63, 052505 (2001)

Demonstration experiment with EUV laser

Absorption length in EUV region



If $I = 10^{13} W/cm^2$

Deposition power

$=> 10^{19} W/cm^3$

Even within 10fs,

$E \sim 10^5 J/cm^3$

$= 10^{11} J/m^3 = 1 Mbar$

ρ = 19.3 g/cc, $h\nu$ = 25eV

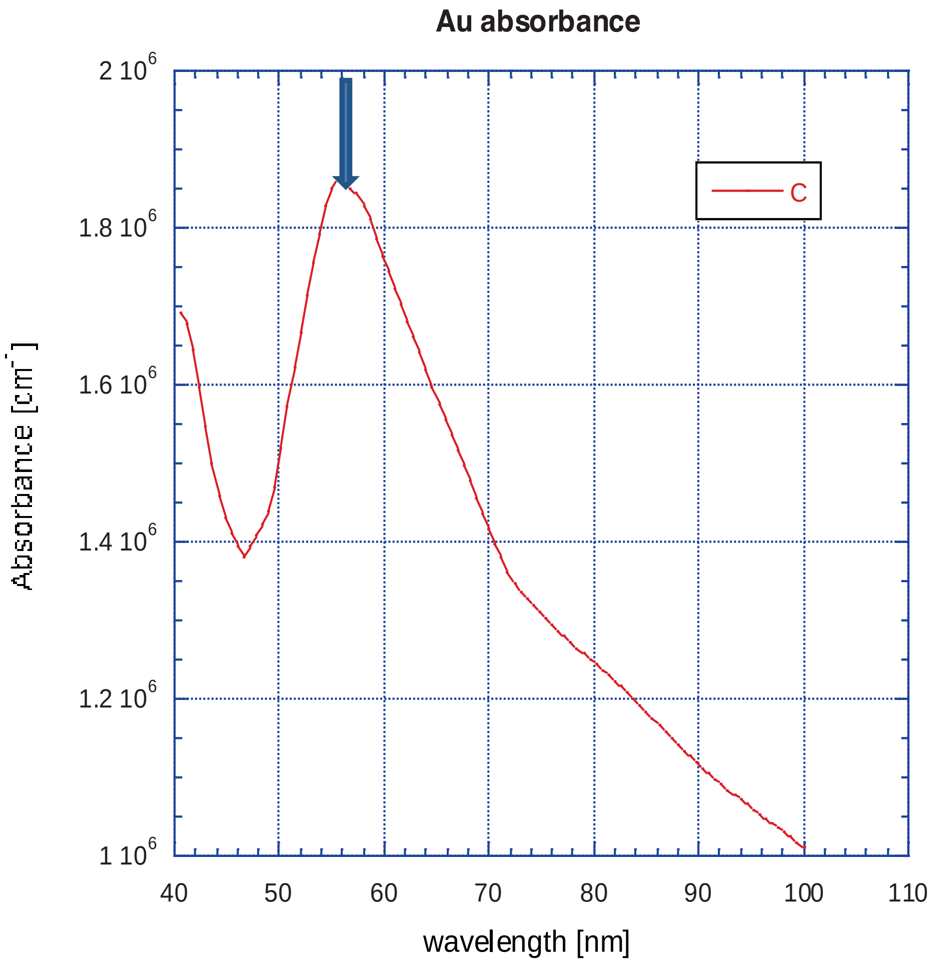
$n_i = 5 \times 10^{22} cm^{-3}$

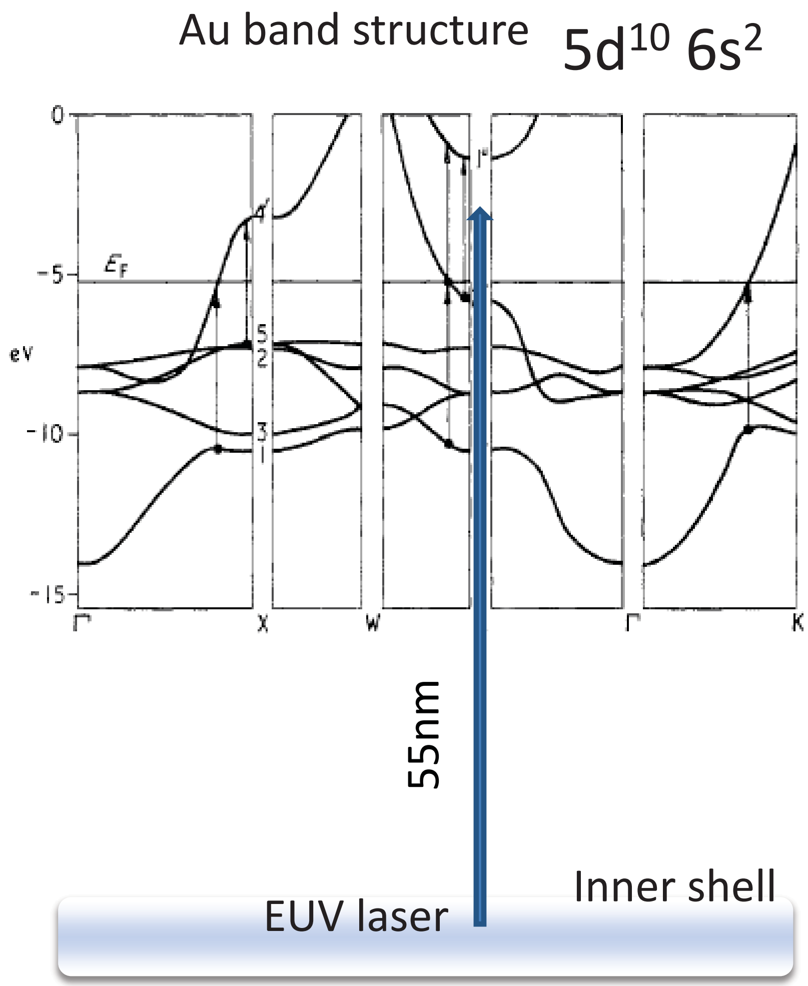
$\alpha = 5 \times 10^6 cm^{-1}$

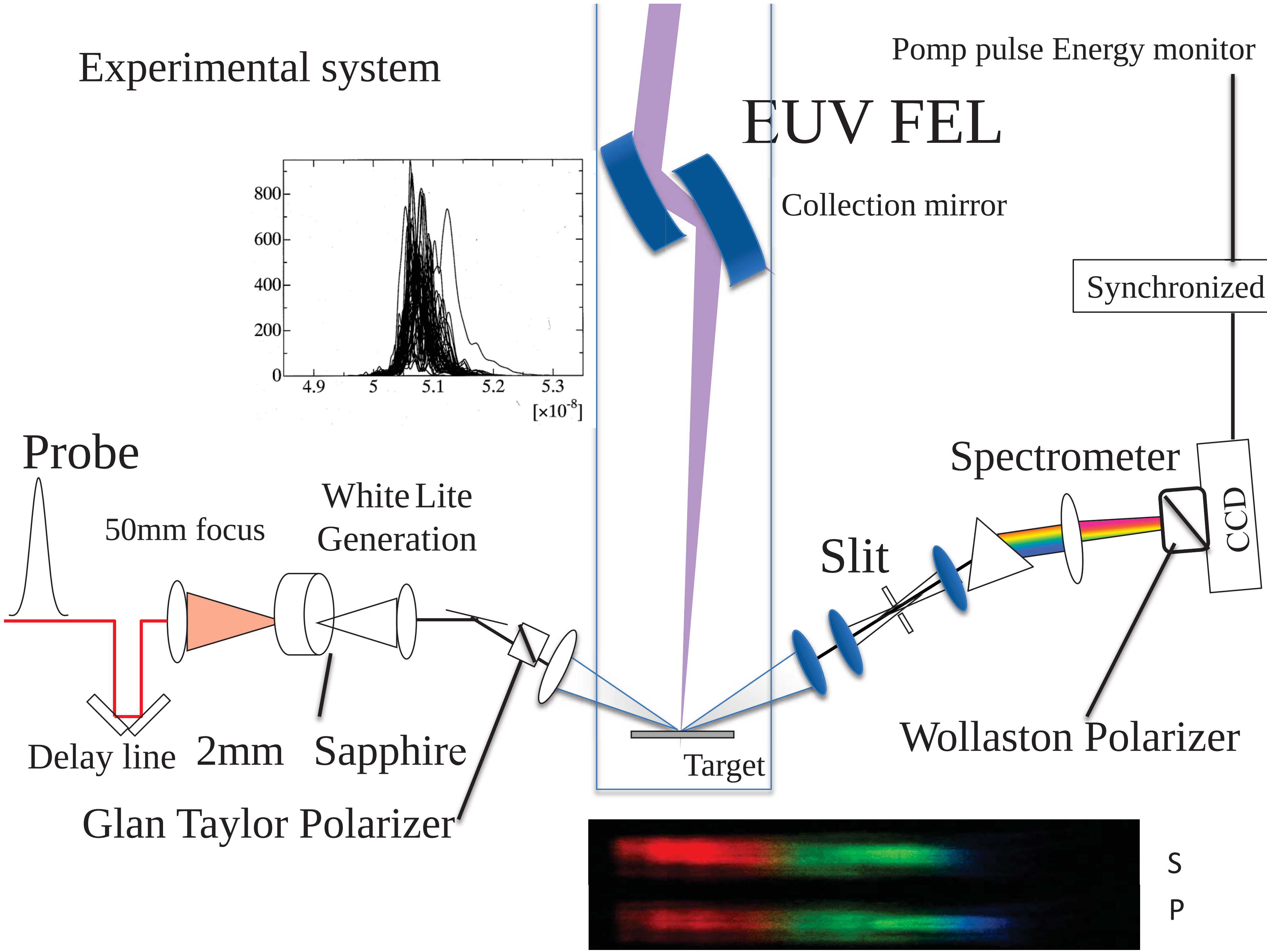
$\tau_{exp} \sim 10 fs$

$(I = 3 \times 10^{13} W/cm^2)$

What is excited state condition of electrons in solid with well-tuned high energy photons?







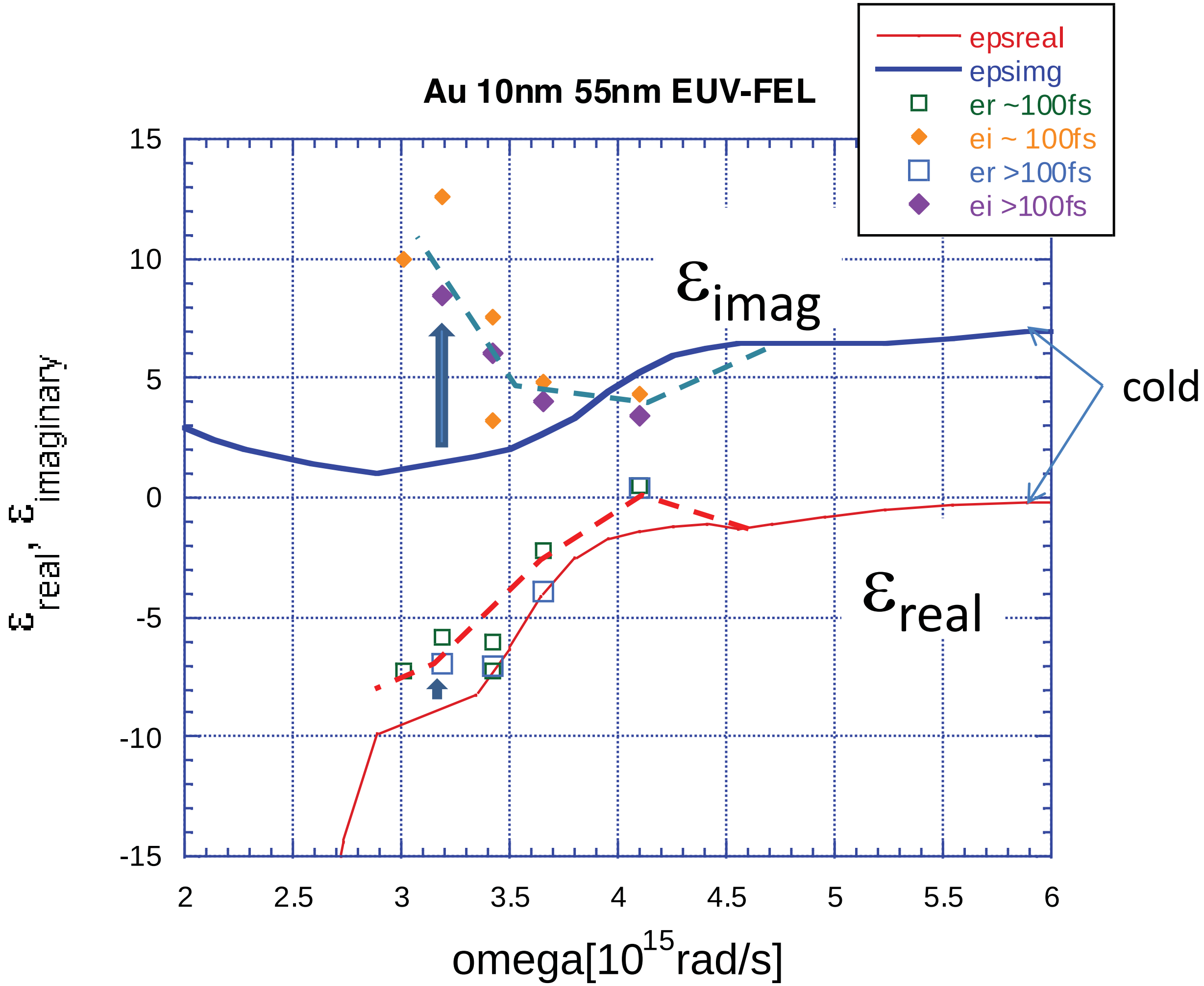
Experimental system
EUV FEL
Pomp pulse Energy monitor
Collection mirror
Synchronized
800
600
400
200
0
4.9
5
5.1
5.2
5.3
[×10-8]
Probe
50mm focus
White Lite
Generation
Spectrometer
CCD
Slit
Delay line
2mm
Sapphire
Target
Wollaston Polarizer
Glan Taylor Polarizer
S
P

Drude ?

$$\epsilon_1 = n^2 - k^2 = \varepsilon_\infty - \frac{{\omega_p}^2}{\omega^2+\gamma^2}$$

$$\epsilon_2 = 2\mathrm{nk} = \frac{{\omega_p}^2}{\omega(\omega^2+\gamma^2)}$$

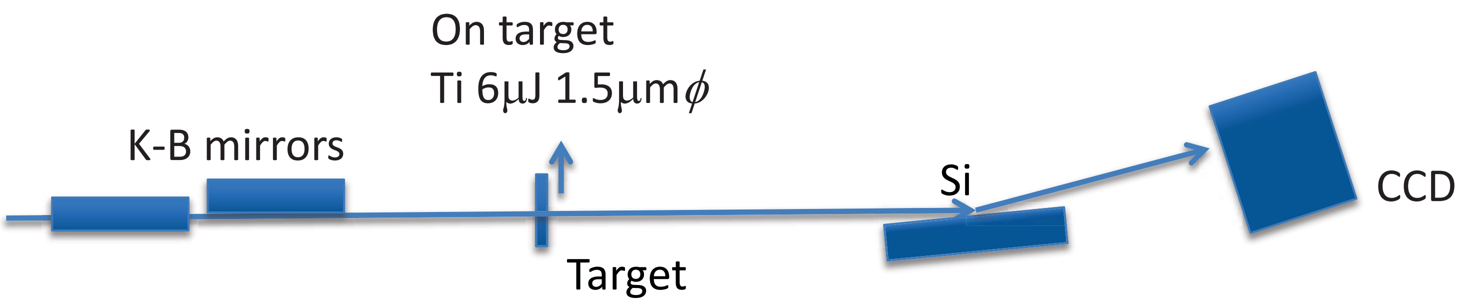
This phenomena is not observed at Ag.

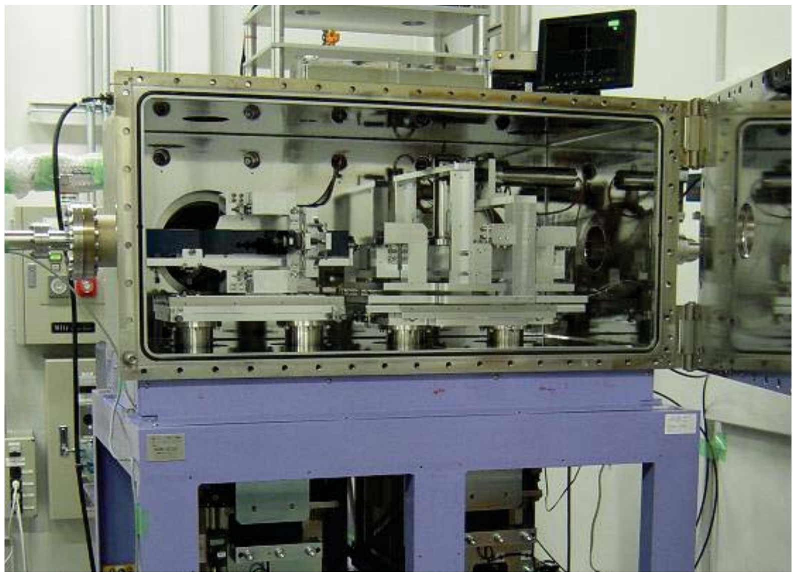


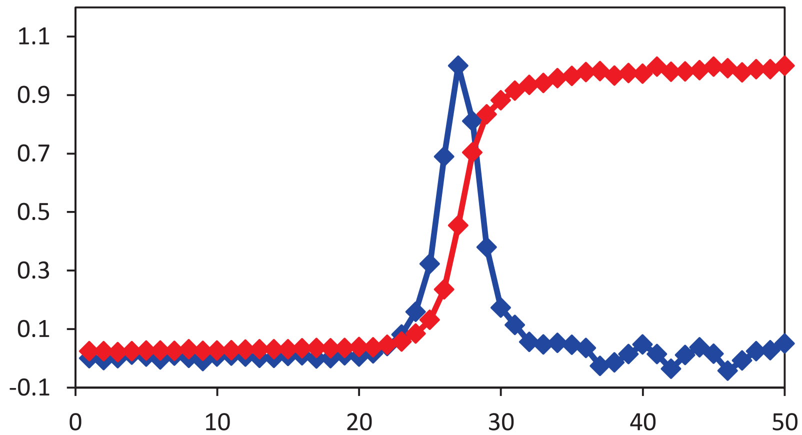
It is NOT free electrons. There are also resonant feature.

Can the photo excitation rate exceed Auger rate in K-shell electrons?

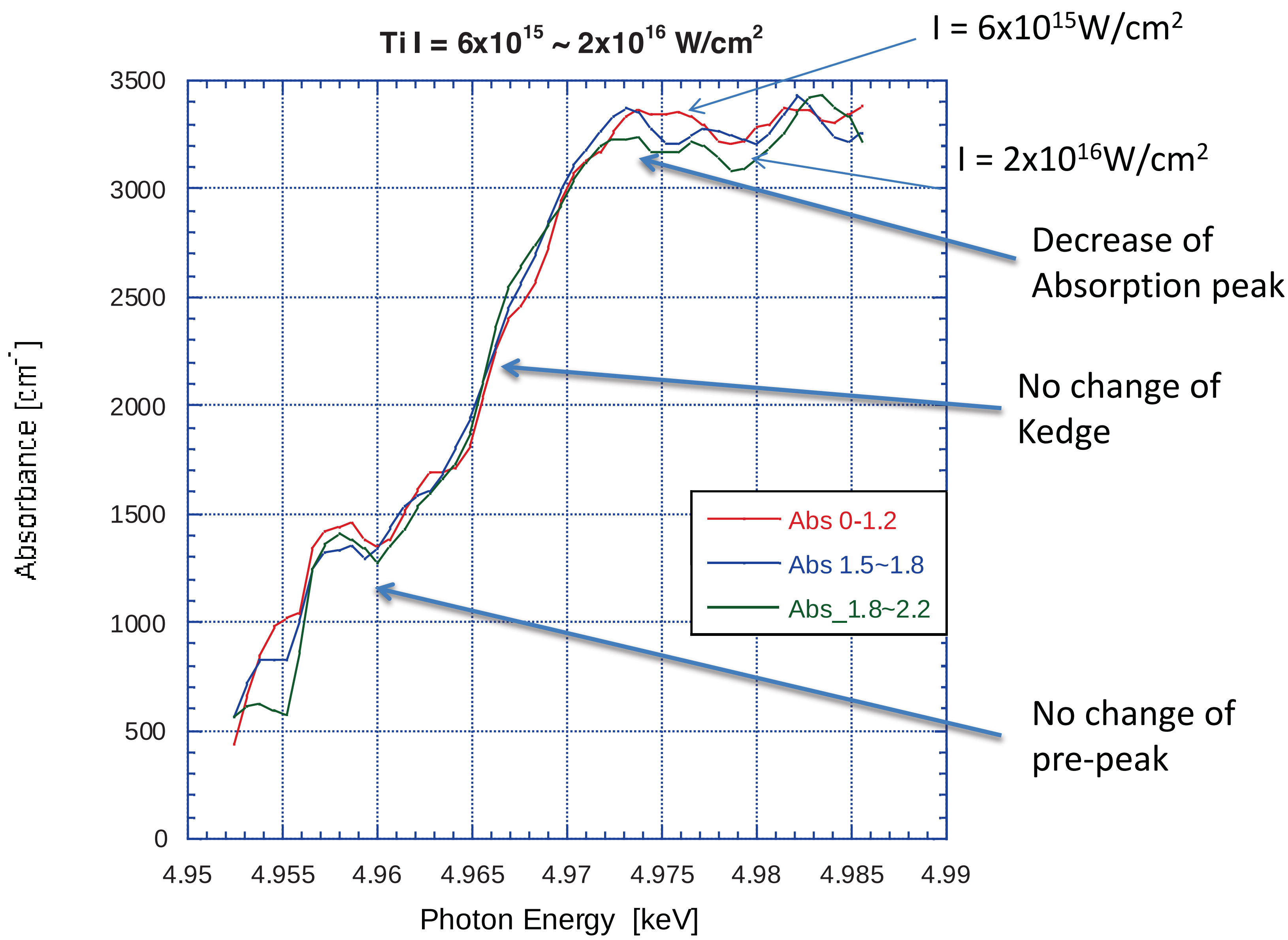
XFEL SACLA experiments





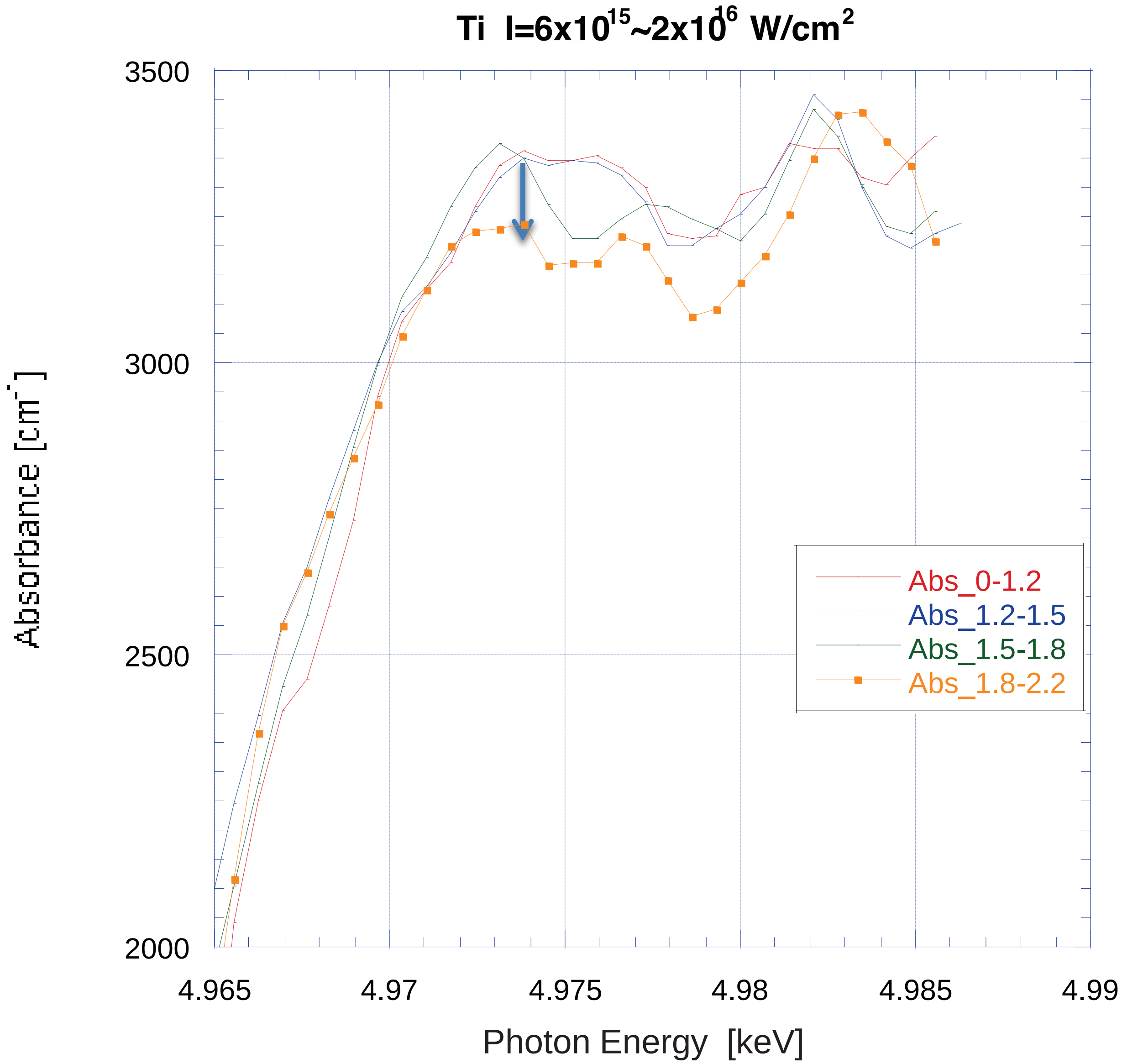


Osaka U: Yamauchi et al, U Tokyo: Mimura et al
SACLA/SP8: Ohashi, Yumoto, Koyama, Tono et al



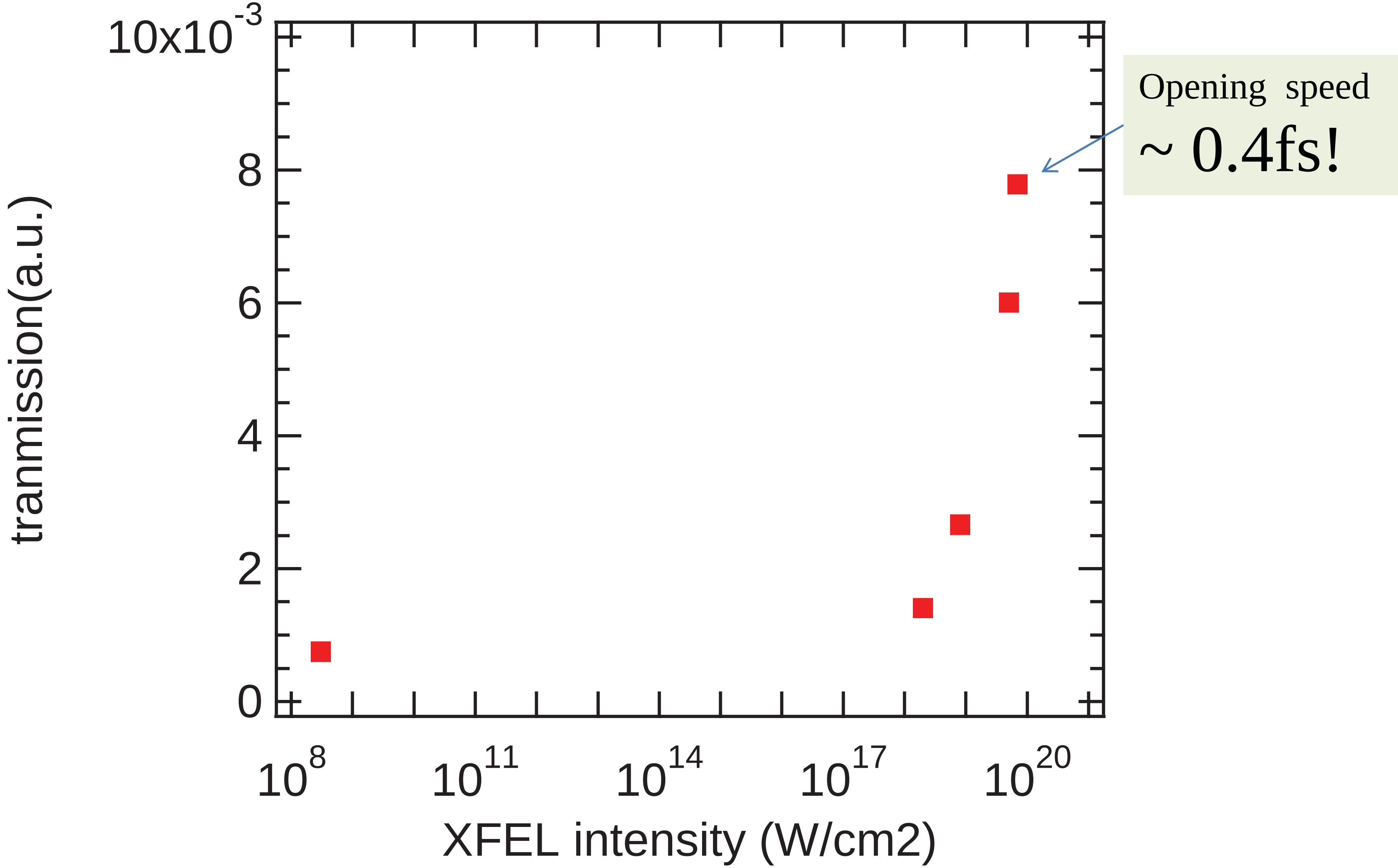
Ti I = 6x10^15 ~ 2x10^16 W/cm^2
I = 6x10^15W/cm^2
I = 2x10^16W/cm^2
Decrease of Absorption peak
No change of Kedge
No change of pre-peak
Abs 0-1.2
Abs 1.5~1.8
Abs_1.8~2.2
Absorbance [cm-]
Photon Energy [keV]
3500
3000
2500
2000
1500
1000
500
0
4.95
4.955
4.96
4.965
4.97
4.975
4.98
4.985
4.99

Transmission spectrum under illumination of intense XFEL

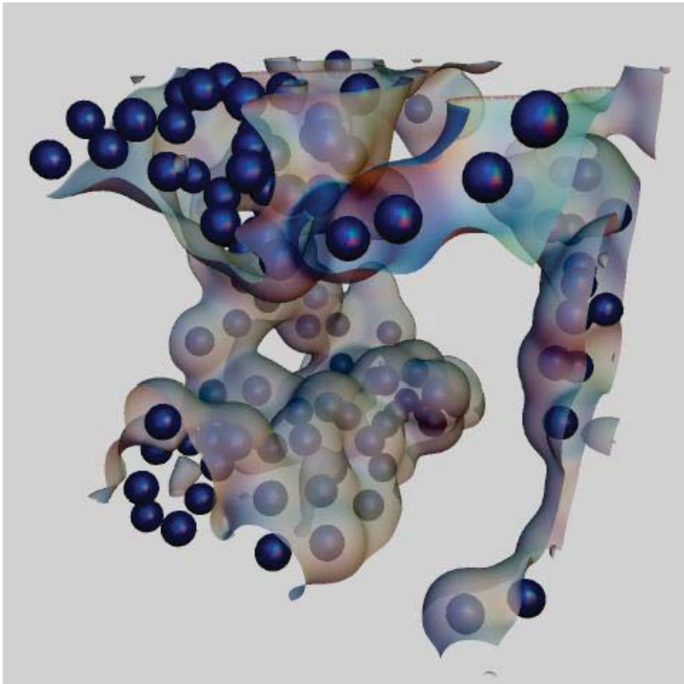


α at Fe K edge ~ 3216cm^{-1} at 7keV

Auger time is 0.9fs



We should measure directly the energy density state of electrons, disordering of ions, transport coefficient (electron, diffusion, thermal….), sound velocity, viscosity, and specific heat.



QMD simulation view of wdm Al, Michael Desjarlais, 2008 WDM school