Warm Dense Matter

Mohammed Shihab

Physics Department, Faculty of Science
Tanta University

Outline

- Introduction.
  - Plasma State
  - Solid State
  - Warm dense matter.

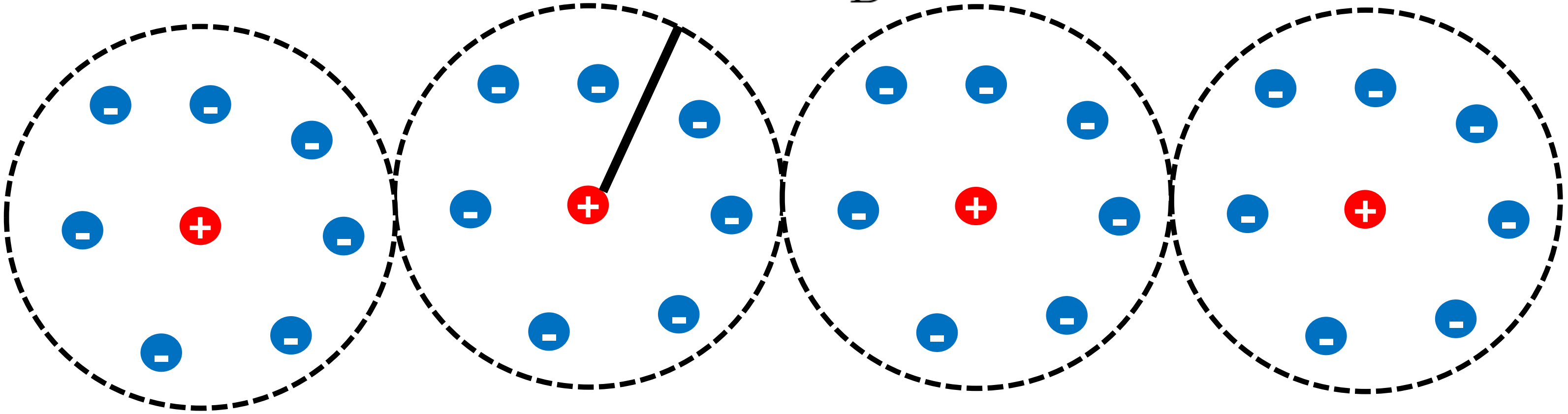
- Warm Dense Matter
  - Motivation behinde the study
  - Generation
  - Invistigation
  - Simulation

- Summary

Debye length

- The Debye radius is the distance at which the potential of an ion charge is decreased by 0.37 of its value in free space.

$$r \approx \lambda_{\mathrm{D}}$$



$$\lambda_{\mathrm{D}} = \sqrt{\frac{\epsilon(K_{\mathrm{B}}T_{\mathrm{e}} + K_{\mathrm{B}}T_{\mathrm{i}})}{Ze^2 n_0}} \quad \Lambda_{\mathrm{D}} = \frac{1}{Zn_0}\left(\frac{\epsilon K_{\mathrm{B}}T_{\mathrm{e}}}{e^2}\right)^{3/2}$$

- In ideal plasma the number of charges Λ_{D} in the Debye sphere must be large.

Debye length

- In a plasma with electron temperature $T_\mathrm{e} = 10000\mathrm{eV}$ and electron density $n_\mathrm{e} = 10^{14}\mathrm{cm}^{-3}$, the number of particles in Debye sphere is 4×10^7.

- In Hot Dense Plasma: the number of particles in Debye sphere is 4 when $T_\mathrm{e} = 100\mathrm{eV}$ and $n_\mathrm{e} = 10^{22}\mathrm{cm}^{-3}$.

- In Warm Dense plasma, the number of charges in Debye sphere might be less than 1.

- Note: WDM does not obey the plasma state theories.

Collision frequency

- In a simple model where ions are assumed to be immobile, the electron ion collision frequency is given as

$$\nu_{\mathrm{ei}} = \frac{8\pi Z^2 e^2 n_{\mathrm{i}}}{3^{3/2} m_{\mathrm{e}}^{1/2} (K_{\mathrm{B}} T_{\mathrm{e}})^{3/2}} \ln \Lambda_c$$

- Coulomb logarithm

$$\Lambda_c = \frac{(K_{\mathrm{B}} T_{\mathrm{e}})^{3/2}}{2Ze^2\sqrt{4\pi e^2 n_{\mathrm{i}}}}$$

- For WDM the collision frequency is negative value.

Conductivity I

- From the generalized Ohm's law

$$I = \frac{1}{R} V \qquad \vec{J} = \sigma \vec{E}$$

- The current density in an ideal plasma is proportional to the applied electric field.

$$\sigma = \frac{e^2 n_\mathrm{e}}{m_\mathrm{e} \nu_\mathrm{ie}} = \frac{3^{1/2}}{8\pi Z e^2 m_\mathrm{e}^{1/2}} \frac{(K_\mathrm{B} T_\mathrm{e})^{3/2}}{\ln(\Lambda_c)}$$

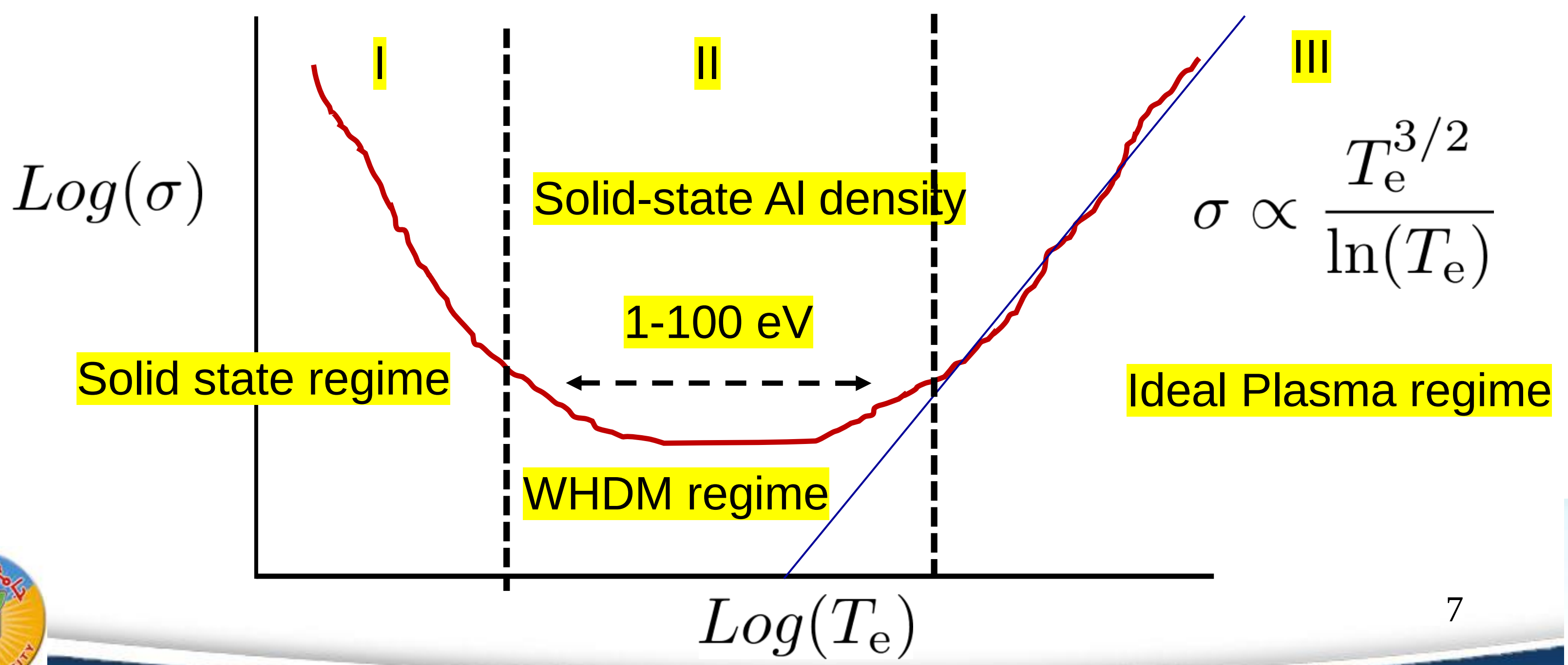
- At constant density:

$$\sigma \propto \frac{T_\mathrm{e}^{3/2}}{\ln(T_\mathrm{e})}$$

Conductivity II

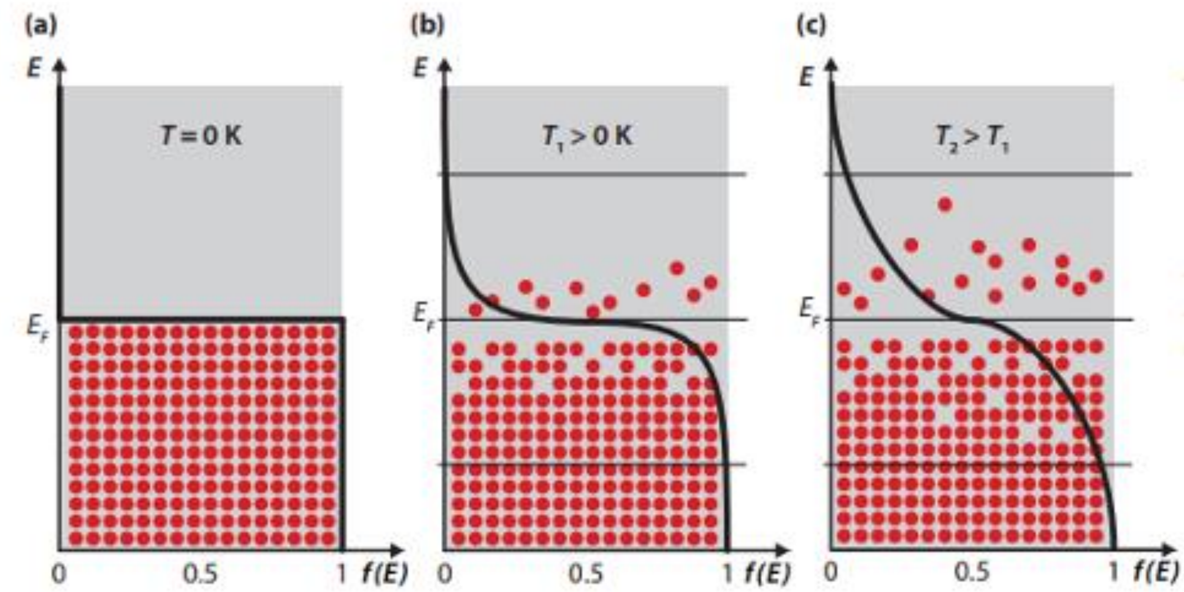
- The plasma conductivity

$$\sigma = \frac{e^2 n_\mathrm{e}}{m_\mathrm{e}\nu_\mathrm{ie}} = \frac{3^{1/2}}{8\pi Z e^2 m_\mathrm{e}^{1/2}} \frac{(K_\mathrm{B} T_\mathrm{e})^{3/2}}{\ln(\Lambda_c)}$$



$$\sigma \propto \frac{T_\mathrm{e}^{3/2}}{\ln(T_\mathrm{e})}$$

Free electron gas theory



- Ferm

$$f(E) = \frac{1}{e^{(E-E_\mathrm{f})}+1} \qquad E_\mathrm{f} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

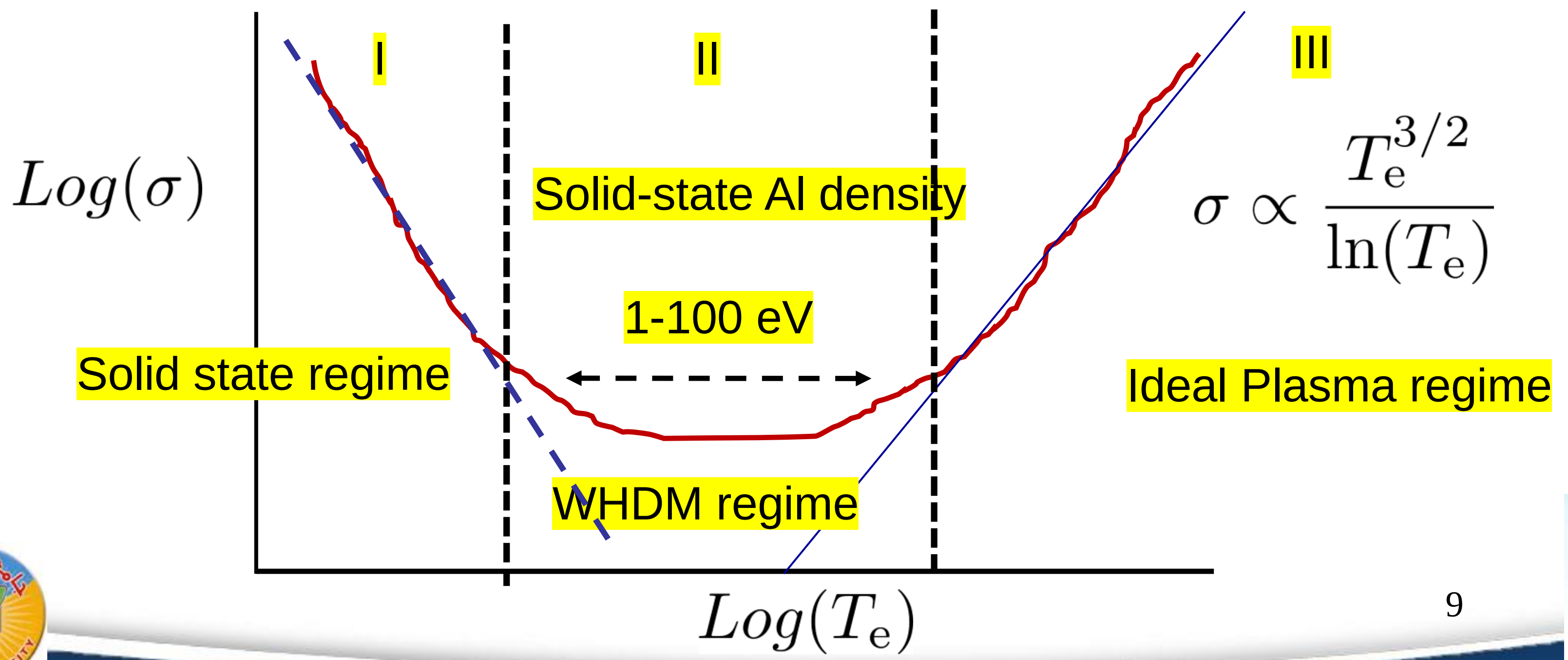
- For solid state density:

$$E_f \approx 2.2eV$$

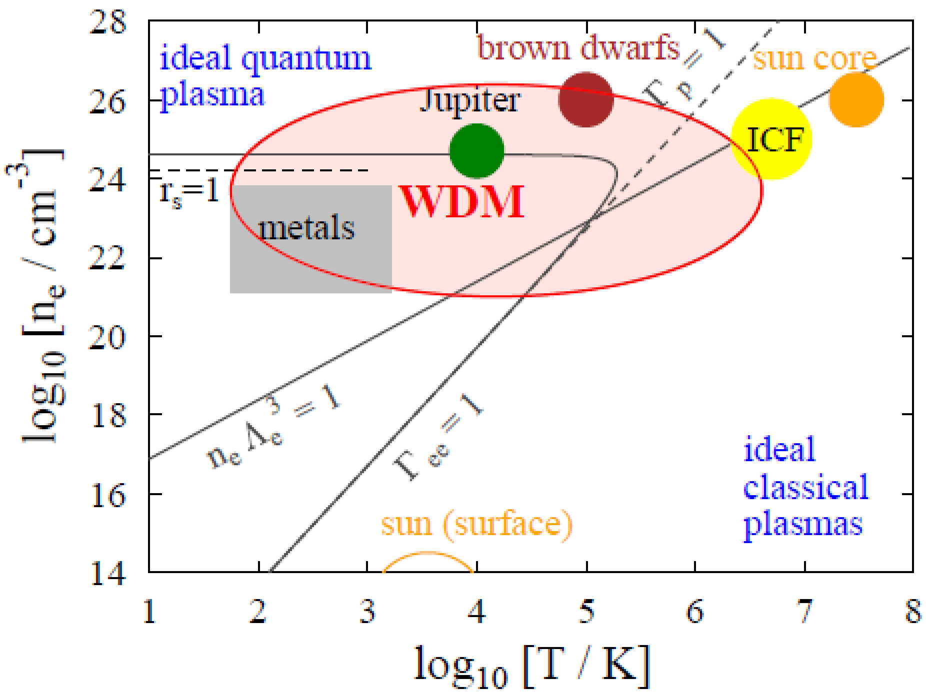
Conductivity III

- The conductivity of a metal decreases by increasing the temperature.

$$\sigma = \frac{e^2 n_\mathrm{e}}{m_\mathrm{e} \nu_\mathrm{ie}} \propto \frac{1}{T}$$



Warm Dense Matter



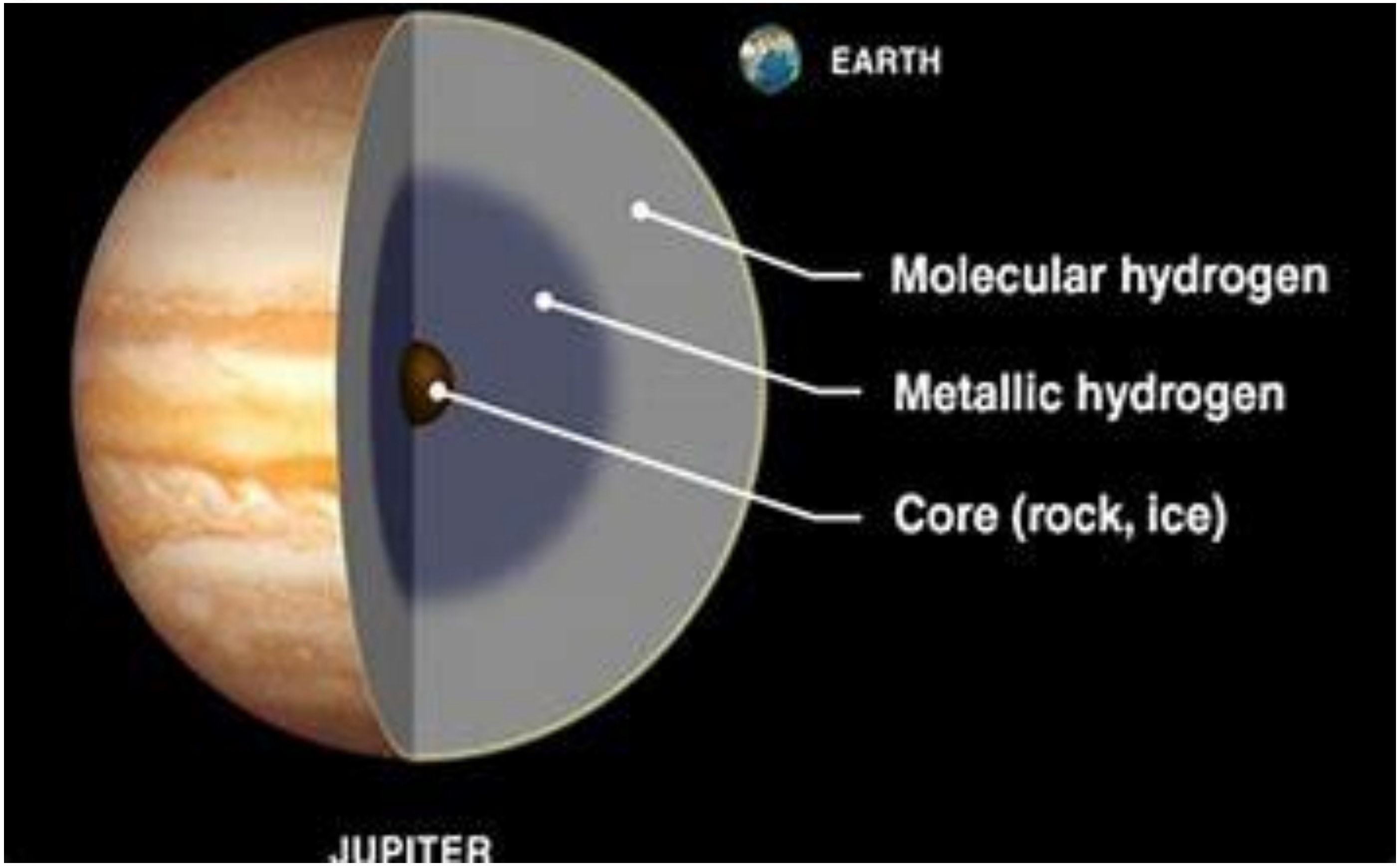
K. Wünsch

- WDM:
  - Temperature of few electronvolts
  - Solid state density and beyond
- ICF, shock experiments, giant planets, and brown dwarfs
- Theories of solid, condensed matter, or ideal plasma are not valid
- No single theoretical model describes the behavior of WDM
  - Partial ionization
  - Arbitrary degeneracy
  - Strong ionic correlations

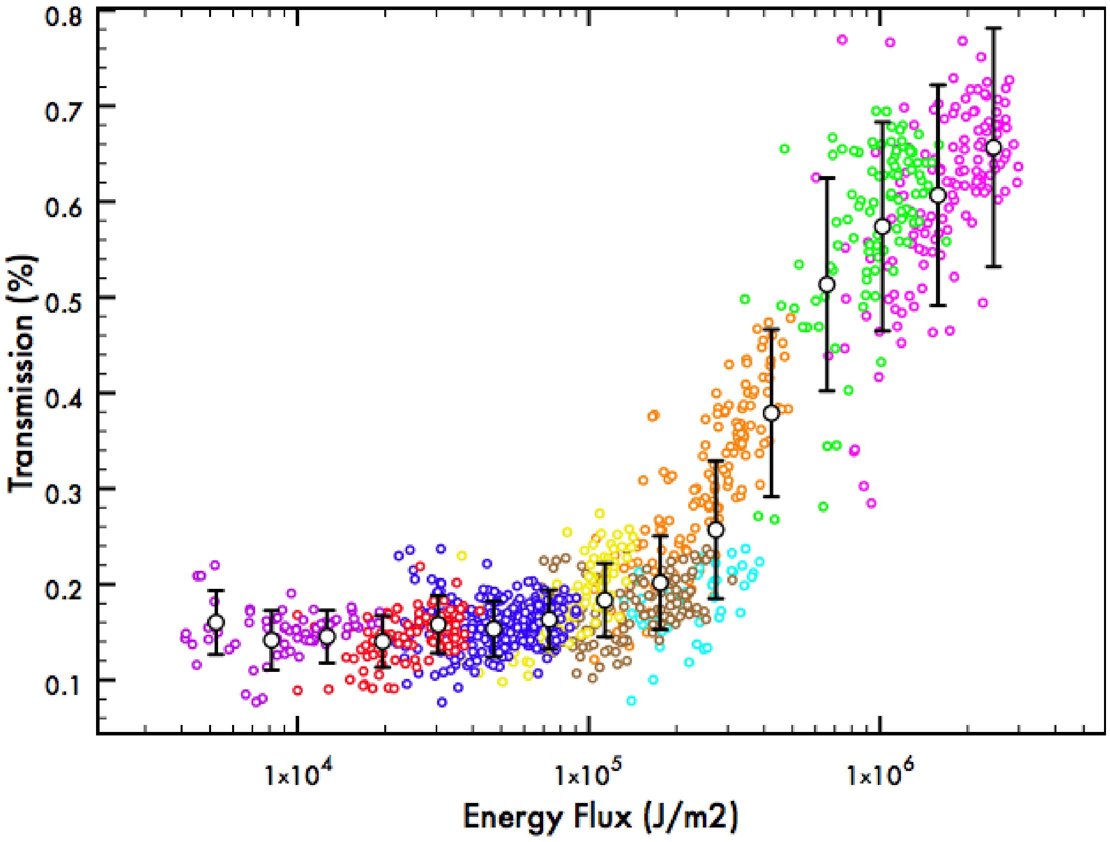
Glenzer et al PRL 98 065002(2007)

WDM in Laboratory

Metallic Hydrogen in Jupiter



Transparent Aluminum



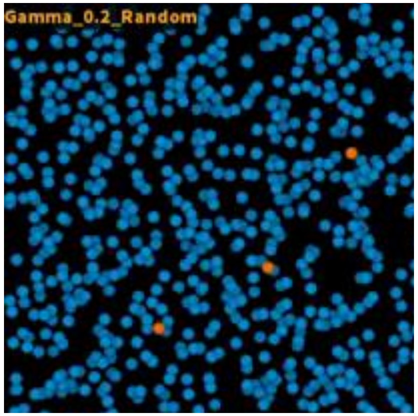
1986

Nagler et al, nature physics 5, 693(2009)

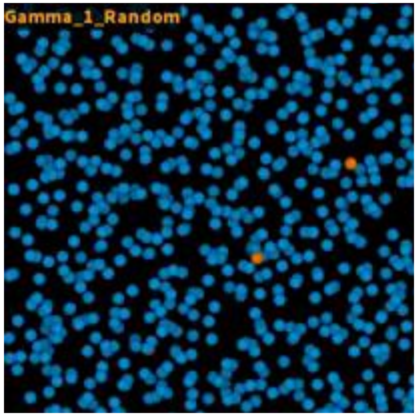
WDM parameters I

- The coupling factor: $$\Gamma = \frac{P.E.}{K.E.} = \frac{e^2}{4\pi\epsilon_0 K_B T_e}\left(\frac{4\pi n_e}{3}\right)^{1/3}$$

$\Gamma = 0.1$

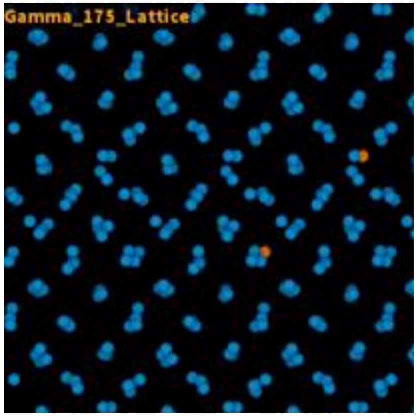


$\Gamma = 1$

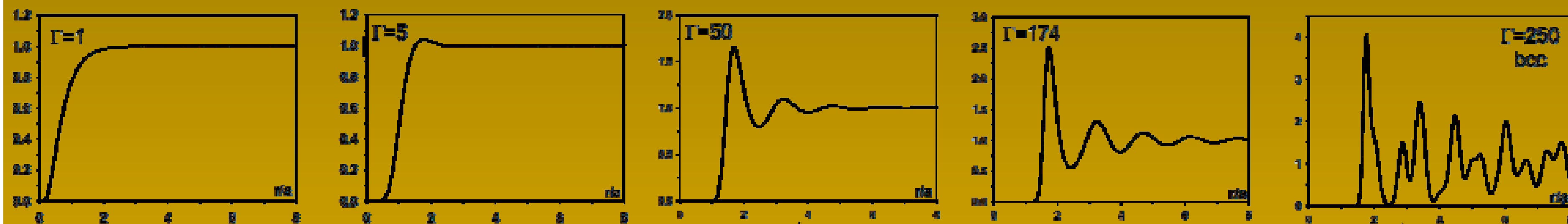


$\Gamma = 50$

$\Gamma = 175$



pair distribution function $g(r)$



WDM parameters II

- The degeneracy factor:

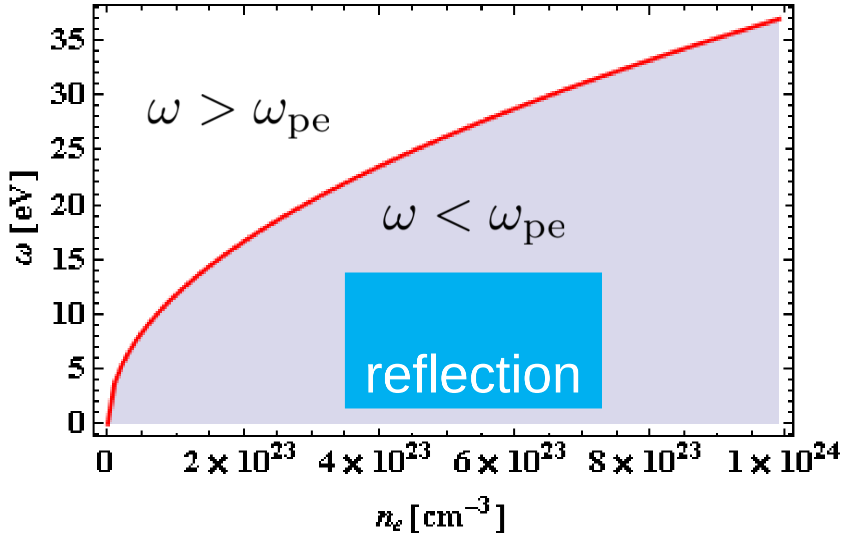
$$\theta_\mathrm{e} = \frac{K_\mathrm{B}T_\mathrm{e}}{E_\mathrm{f}} = \frac{2m_\mathrm{e}K_\mathrm{B}T_\mathrm{e}}{\hbar^2}(3\pi^2 n_\mathrm{e})^{-2/3}$$

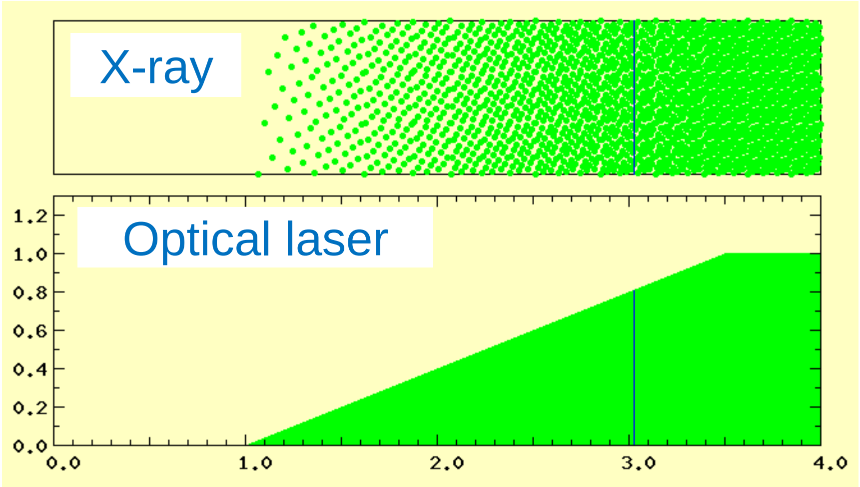
- When $\theta_\mathrm{e} < 1$, most electrons populate states in Fermi see. Quantum effects are important.

- The screening length or Debye length must be calculated from Fermi distribution not form Maxwell-Boltzmann distribution like in ideal plasma.

$$\lambda_\mathrm{D}^{-2} = \frac{e^2 m_\mathrm{e}^{3/2}}{\sqrt{2}\pi^2\epsilon_0\hbar^3}\int dE E^{-1/2} f(E)$$

Dispersion relation of EM in WDM





Warwick UK

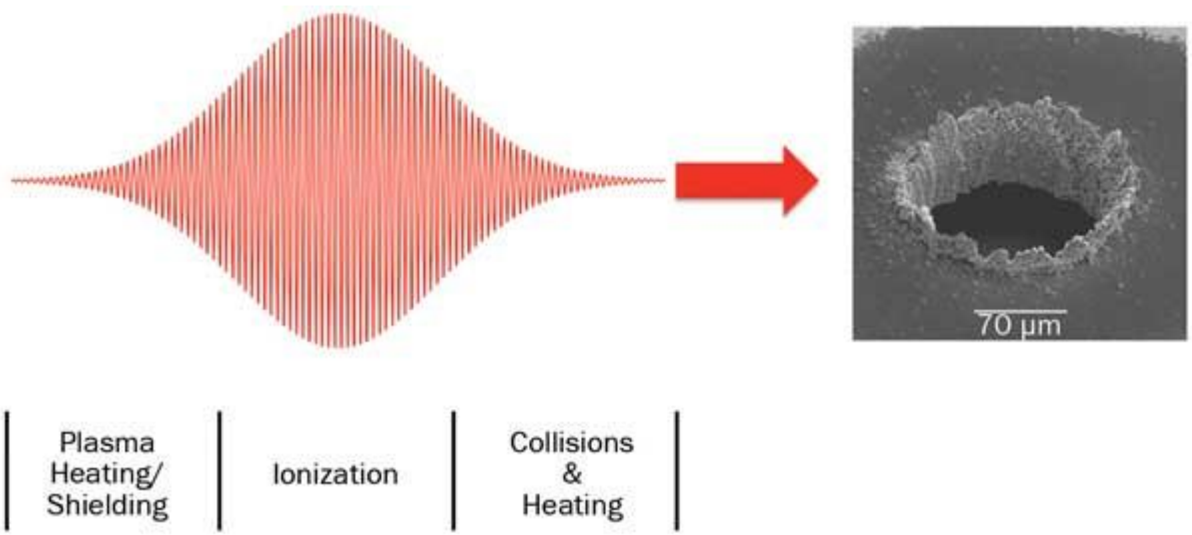
- At the natural plasma oscillation: $\omega_{\mathrm{pe}} = \omega \rightarrow k = 0$

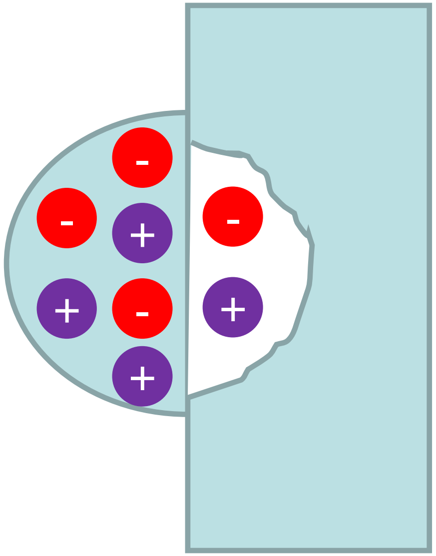
- At the cut off, the wave is reflected: $\omega_{\mathrm{pe}} > \omega \rightarrow k = i\kappa$
- WDM is transparent in x-ray regime:

$$n_{\mathrm{e}} = 10^{24}\mathrm{cm}^{-3} \rightarrow \lambda \leq 33nm$$

Plasma creation over solid targets

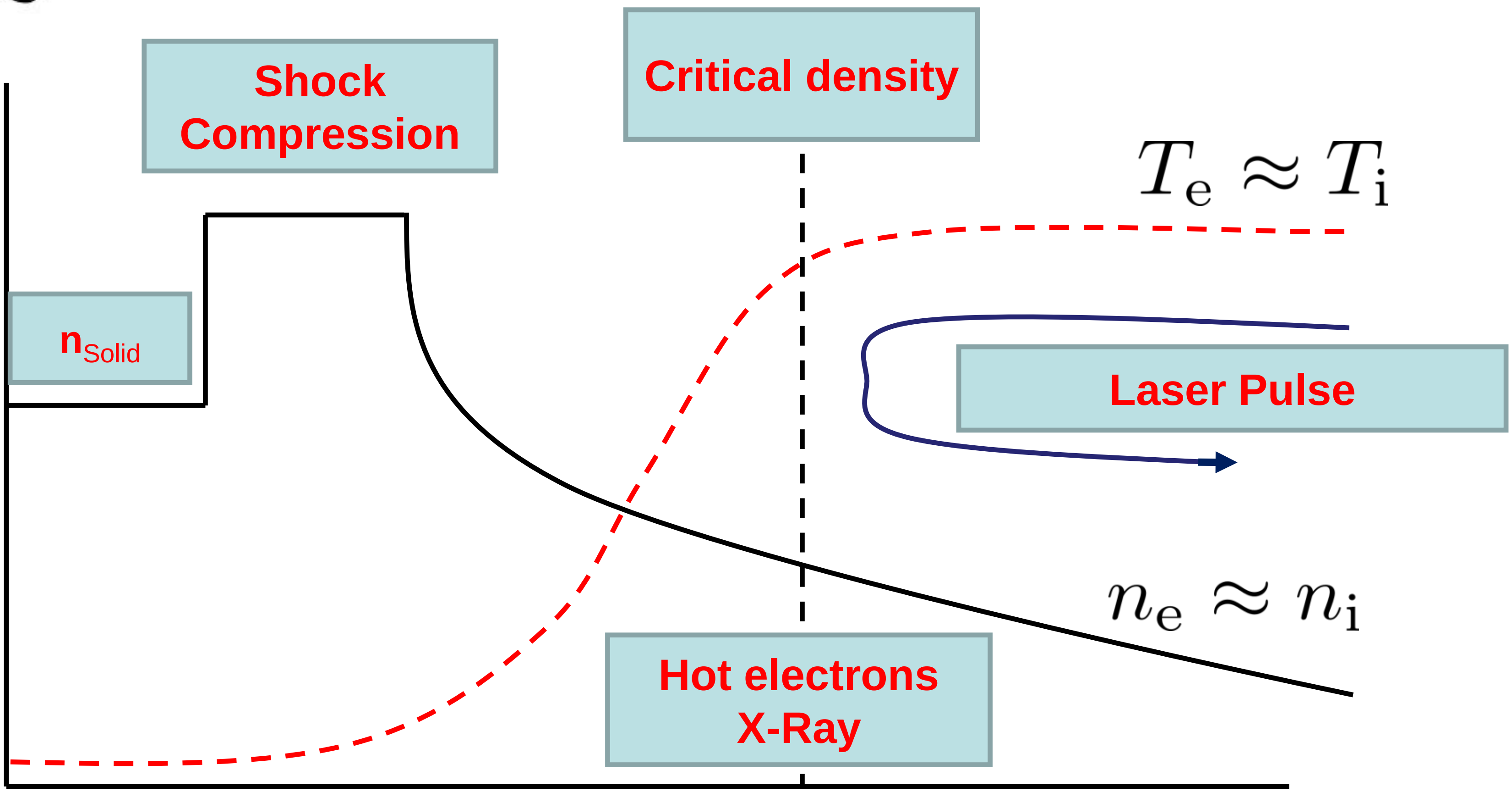
- The first seed of electrons are generated via MPI, Tunnel ionization, or , BSI.
- The free electrons gain energy from the laser electric field, then make further ionization by collision with neutral particles in the target.



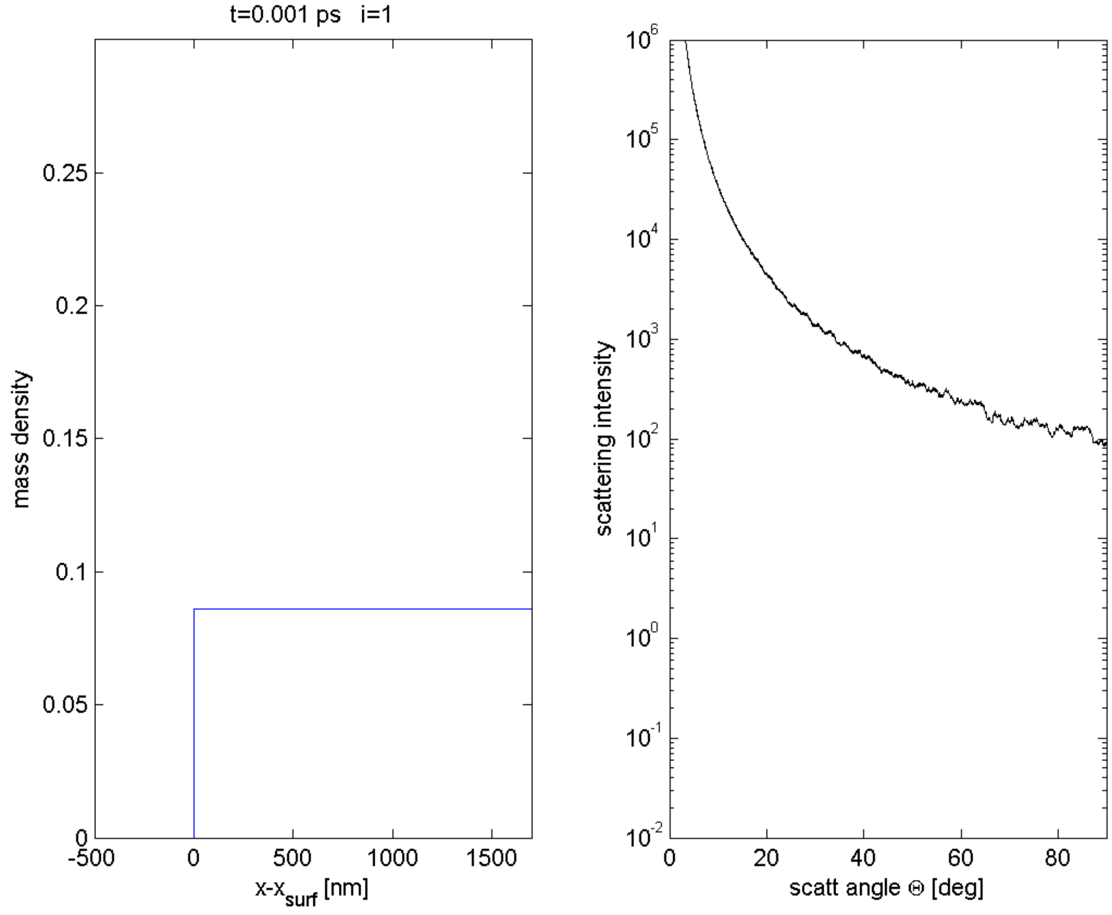


Photonics.com

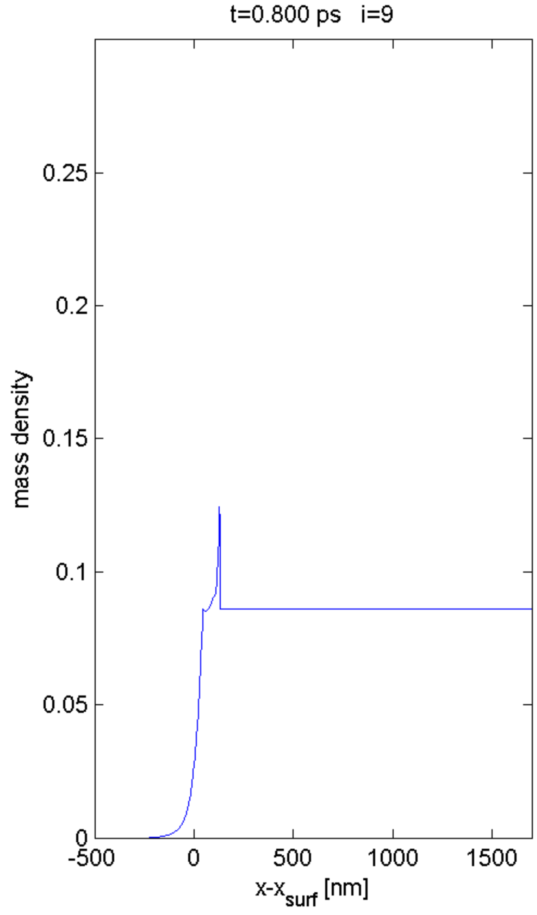
Nano-second optical laser

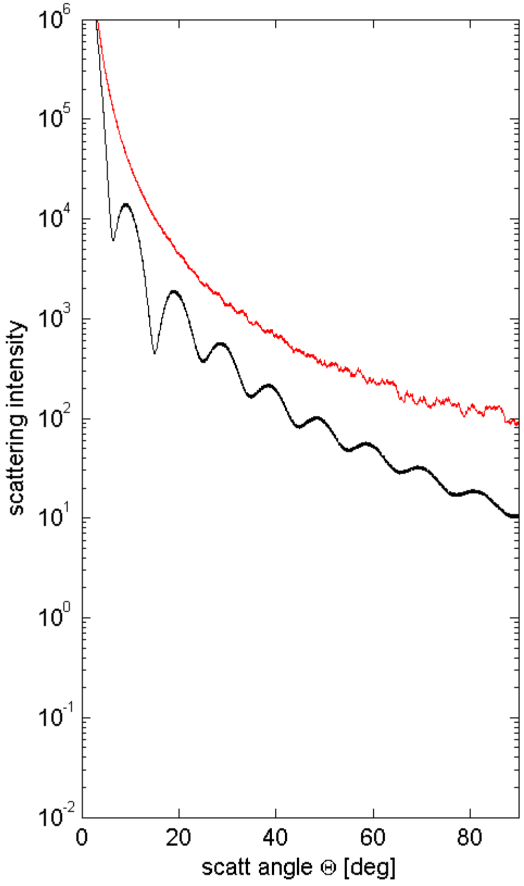


Shock waves and compression

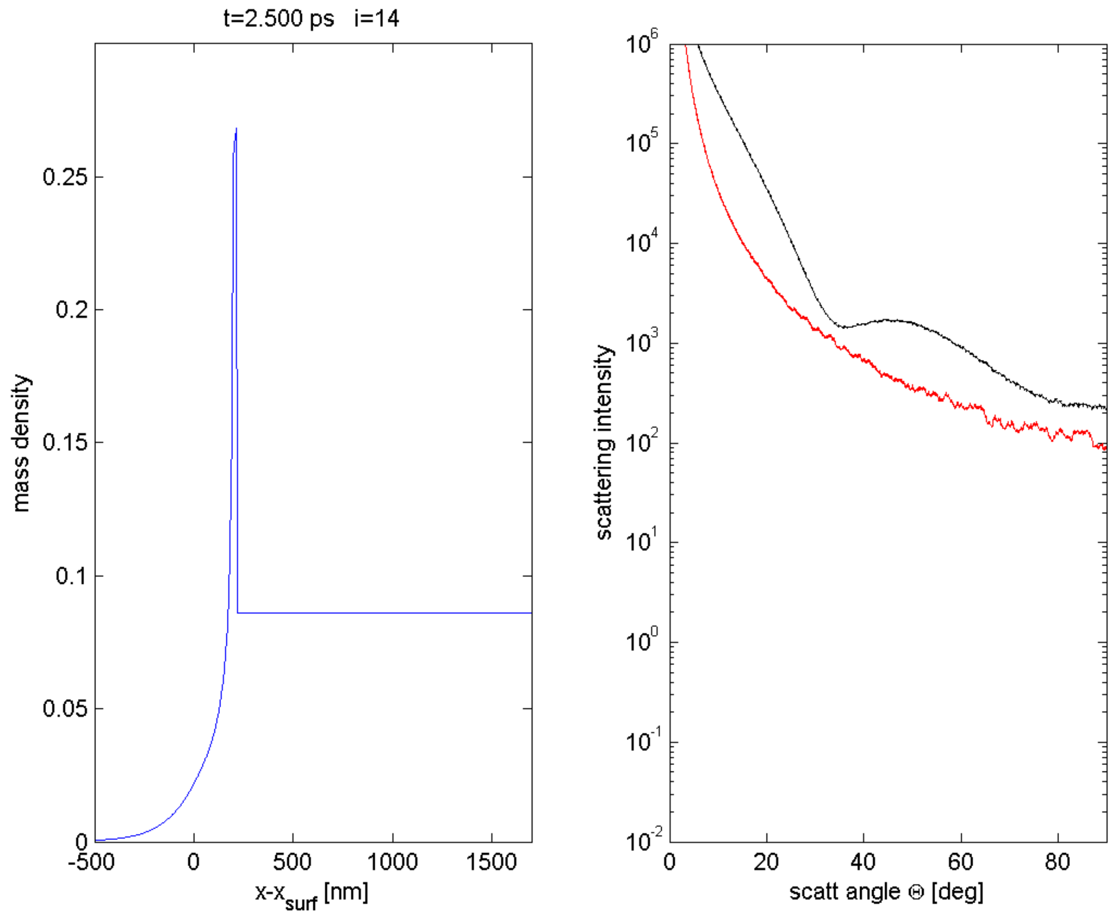


Shock waves and compression

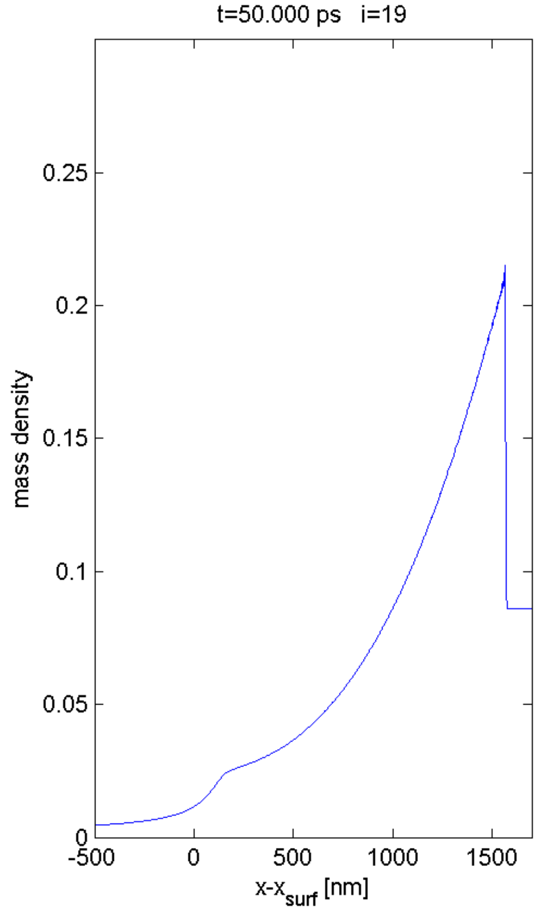


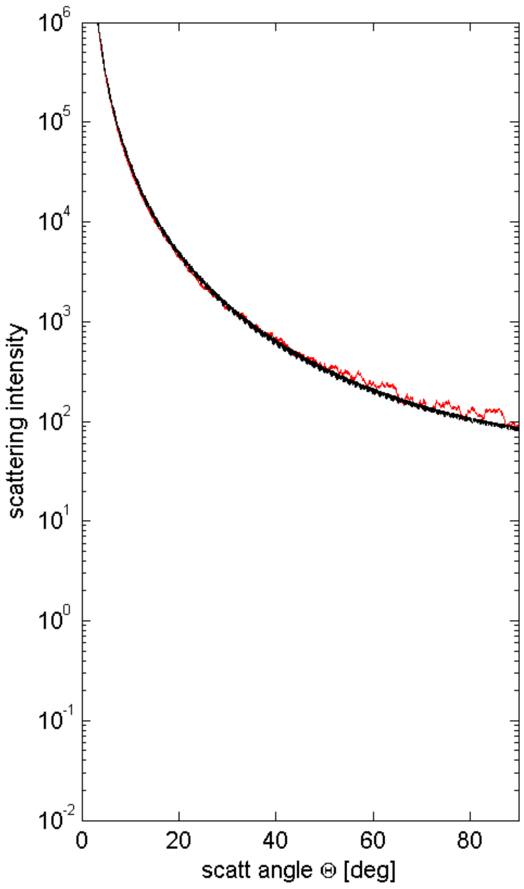


Shock waves and compression

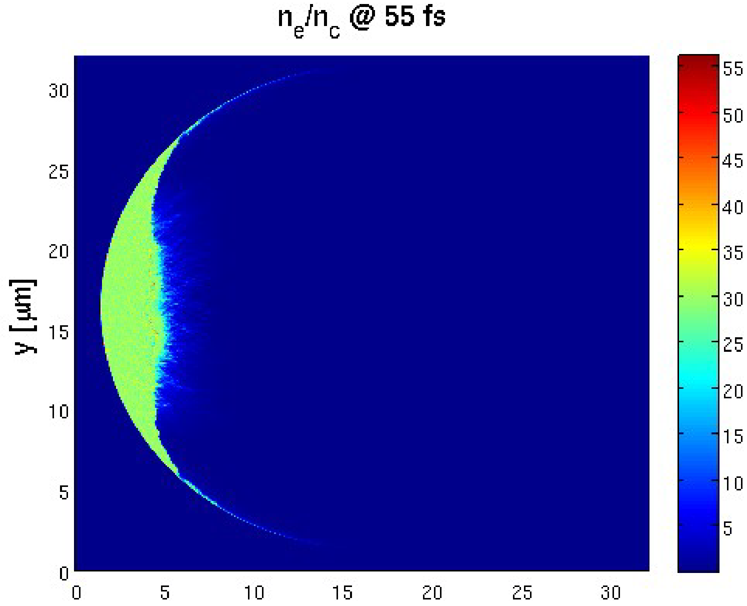


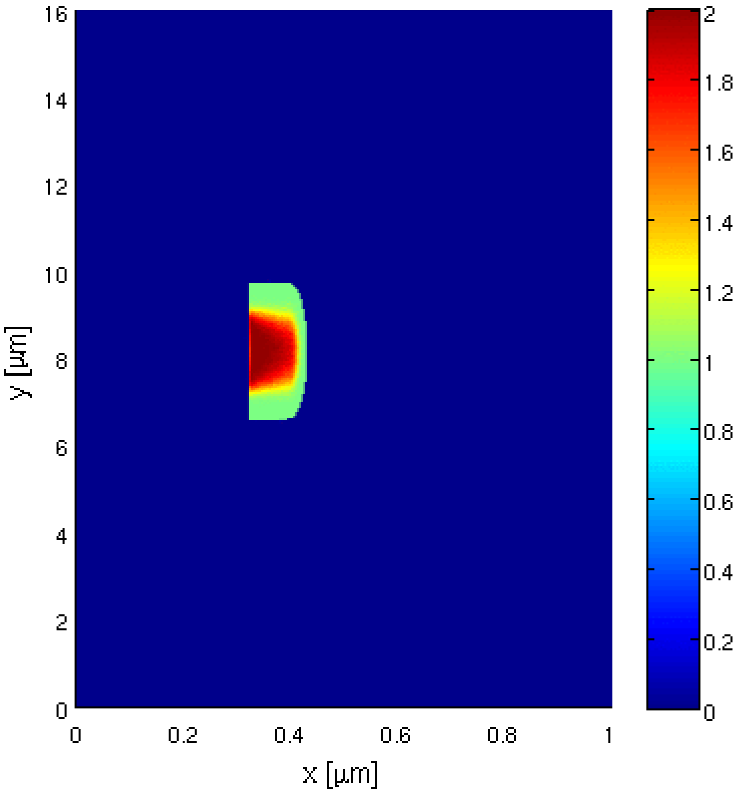
Shock waves and compression



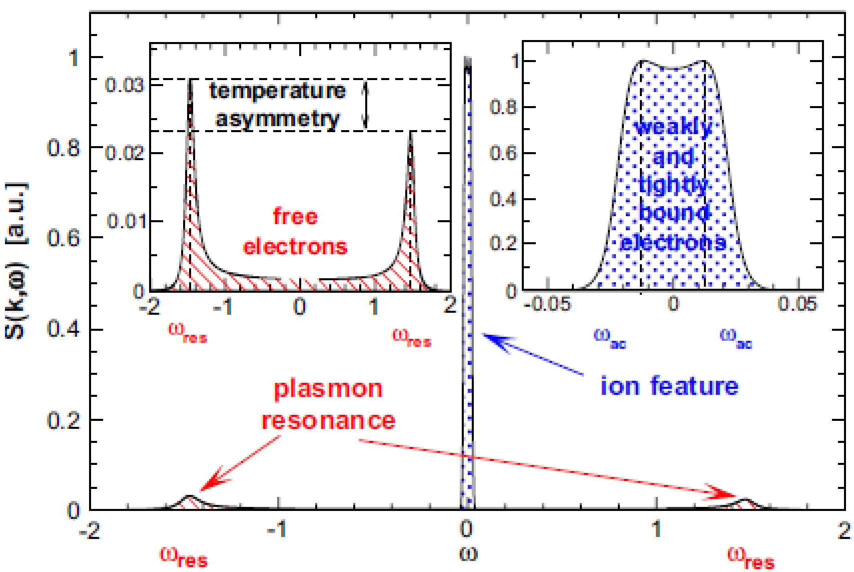


Surface waves





X-ray Thomson scattering



A. Höll et al., HEDP 3, 120(2007)

- Thomson scattering has two distinct features:
  - Inelastic scattering (frequency shifted) from free electrons and bound free transitions
  - Unshifted Rayleigh peak (elastic) due to electrons co-moving with the ions
- The electrons in partially ioized system can be split into bound and free electrons

$$\rho_{\rm e} = \rho_{\rm b} + \rho_{\rm f}$$

- Intermediate scattering function

$$N_{\rm e} F_{\rm ee}^{tot} = \langle \rho_{\rm b}(\vec{k},t)\rho_{\rm b}(-\vec{k},t)\rangle + 2\langle \rho_{\rm f}(\vec{k},t)\rho_{\rm b}(-\vec{k},t)\rangle + \langle \rho_{\rm f}(\vec{k},t)\rho_{\rm f}(-\vec{k},t)\rangle$$

Born-Mermin approximation

- Fluctuation-dissipation theorem :

$$S^0_{\mathrm{ee}}(k,\omega) = -\frac{\epsilon_0 \hbar k^2}{\pi e^2 n_{\mathrm{e}}} \frac{\mathrm{Im}\epsilon^{-1}(\mathrm{k},\omega)}{1-\exp(-\hbar\omega/k_{\mathrm{B}}T_{\mathrm{e}})}$$

- RPA gien by Lindhard:

$$\epsilon^{\mathrm{RPA}}(\vec{k},\omega) = 1 - \frac{1}{\epsilon_0 \Omega_0 k^2} \sum_p e^2 \frac{f^e_{p+k/2} - f^e_{p-k/2}}{\Delta E^e_{p,k} - \hbar(i\omega + i\eta)}$$

- Mermin ansatz :

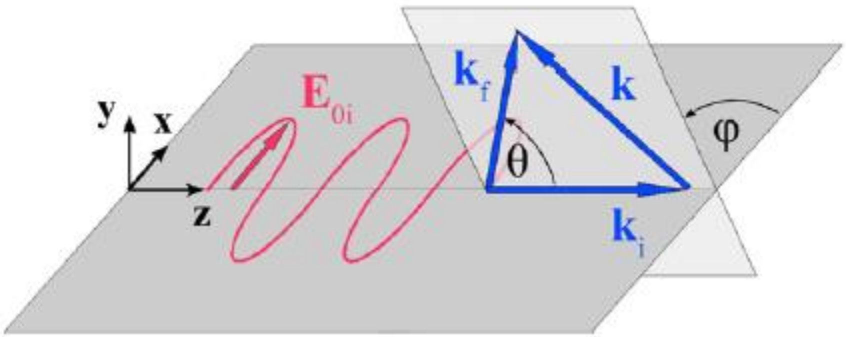
$$\epsilon_M(k,\omega) = 1 + \frac{\left(1+\frac{i\nu(\omega)}{\omega}\right)\left[\epsilon^{\mathrm{RPA}}(k,\omega+i\nu(\omega)) - 1\right]}{1 + i\frac{\nu(\omega)}{\omega}\frac{\epsilon^{\mathrm{RPA}}(k,\omega+i\nu(\omega))-1}{\epsilon^{\mathrm{RPA}}(k,0)-1}}$$

- $\nu(\omega)$ is the dynamic collision frequency via Born approximation.

Glenzer and Redmer, RMP 81, 1625(2009)

Back and forward scattering

- Dimensionless scattering parameter $$\alpha = \frac{1}{k\lambda_{\mathrm{sc}}} = \frac{l}{2\pi\lambda_{\mathrm{sc}}}$$
  - l is the electron density fluctuation
  - λ_{sc} is the screening length
- Collective scattering: ($\alpha > 1$)
  - the scattering reflects the electron density fluctuations
  - Plasmon features
- Non-collective scattering:($\alpha < 1$)
  - the scattering reflects the velocity distribution of electrons
  - Compton features

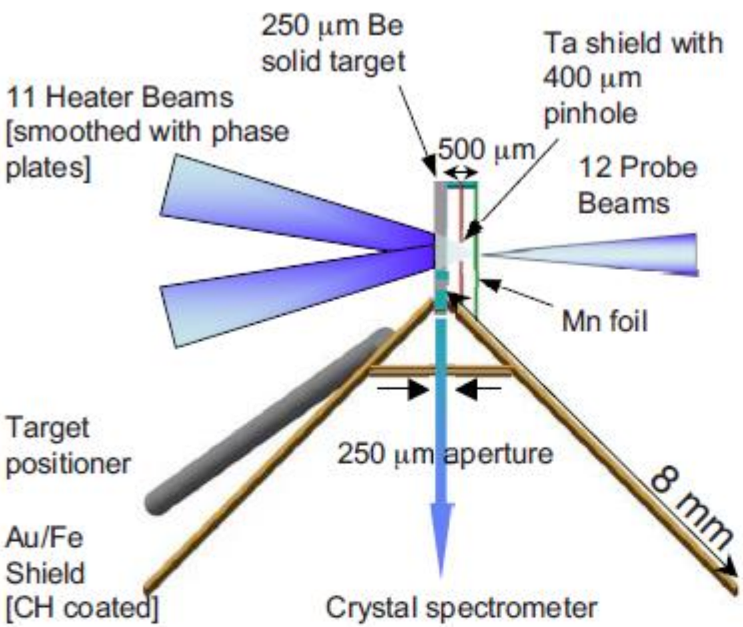


- The momentum transfer depends on the scattering angle

$$k = |k_{\mathrm{f}} - k_{\mathrm{i}}| = \frac{4\pi}{\lambda_{\mathrm{i}}} sin(\theta/2)$$

Glenzer and Redmer, RMP 81, 1625(2009)

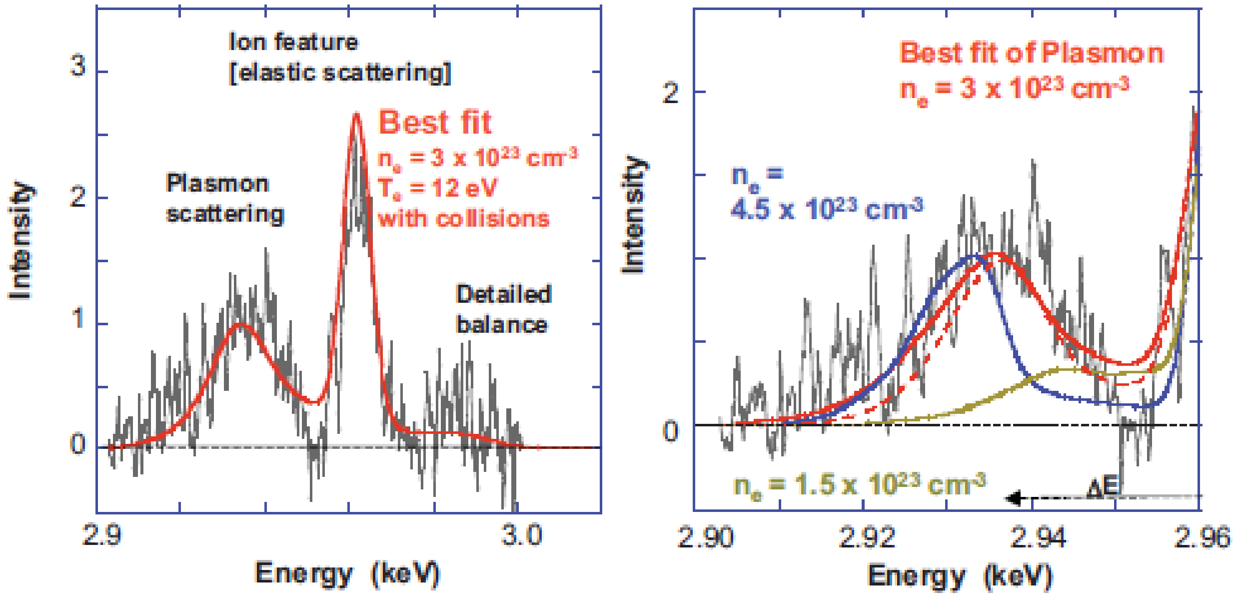
Set up of an experiment



- The target is heated and compressed via laser beams
- Laser beams launch shock waves
- Pressure inside the target in the range of $20 < P < 35$ Mbar
- A backlighters (probe laser pulse) irradiate a Mn target to produce a Mn-He- α line
- x-ray (6.2 KeV) penetrates the target and scattered off the target

H.J. Lee et al., PRL 102, 115001 (2009)

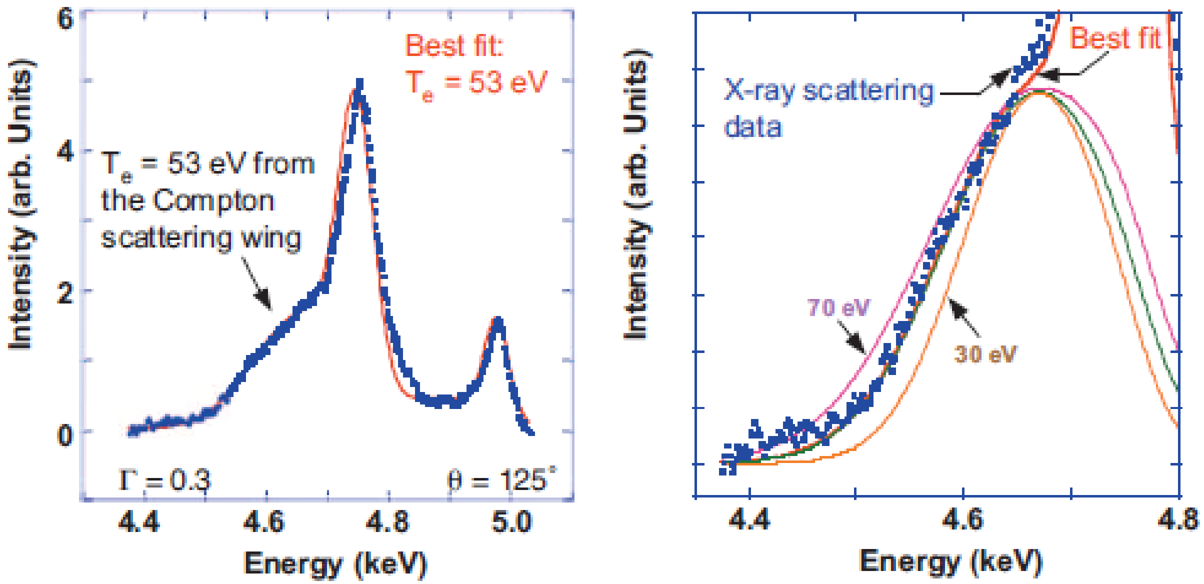
Experimental results and



- **Forward scattering:** collective behavior
- Dispersion relation determines the electron density
- Detailed balance gives the electron temperature

Glenzer et al., PRL 98, 065002(2007)

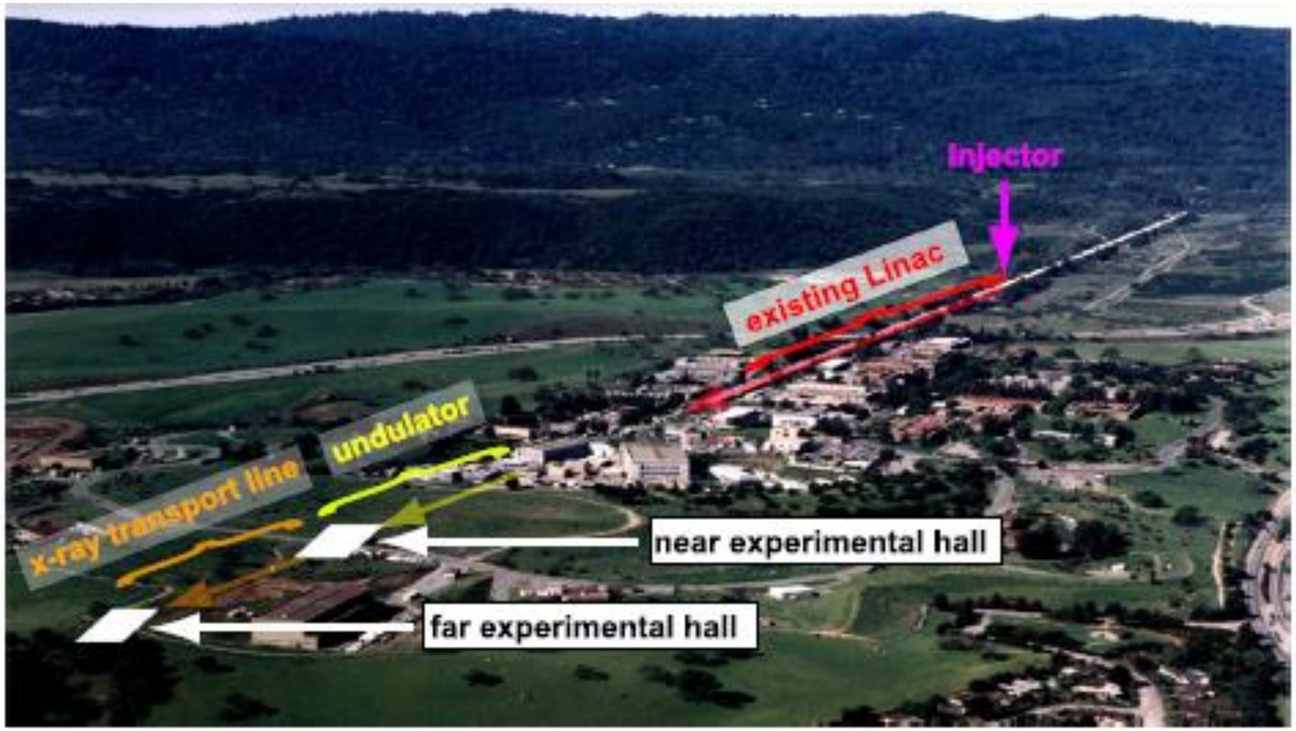
Experimental results and synthetic spectra II



- **Back scattering:**
  - Compton scattering
  - Non-collective behavior
  - Line width $\propto$ Fermi energy

Glenzer et al., PRL 90, 175002(2003)

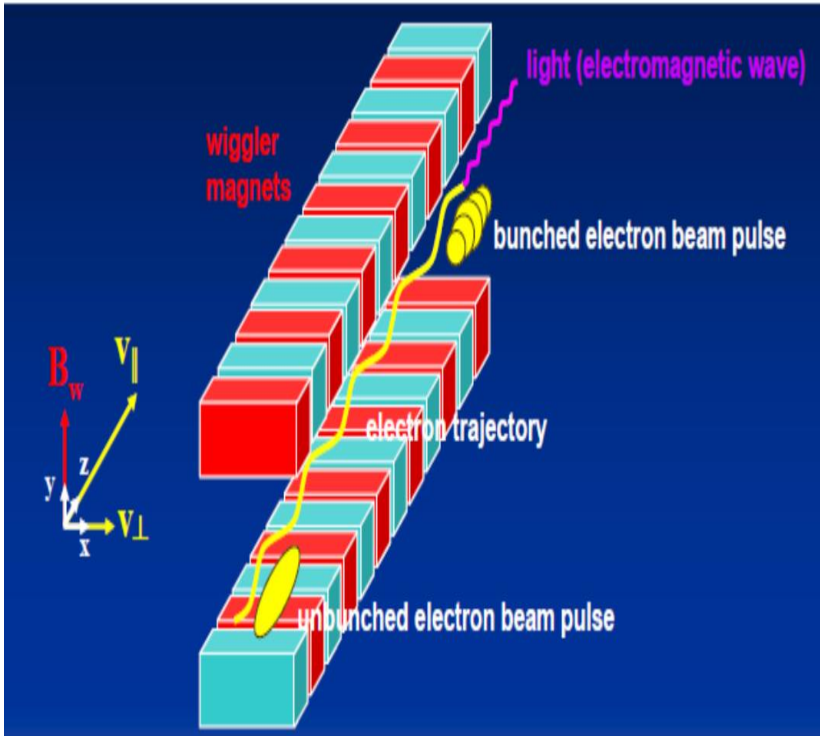
XRFEL experiment



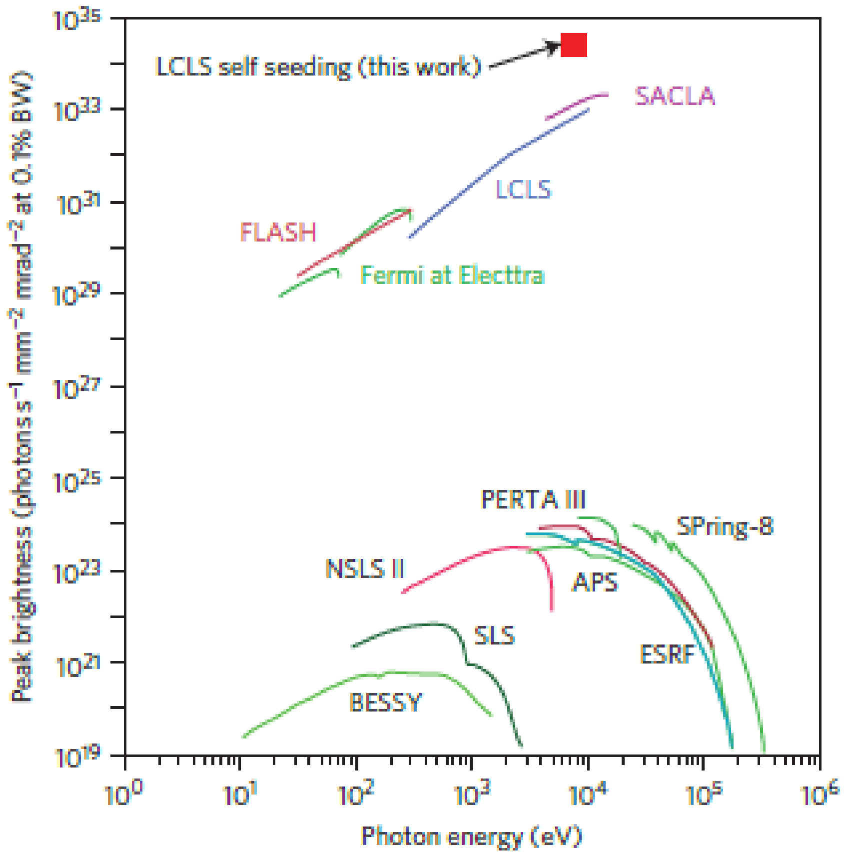
S.H. Glenzer et al., (2016): Stanford University

Free electron laser

- ❖The free electron laser (FEL) is a device that transforms the kinetic energy of a relativistic electron beam into electromagnetic (EM) radiation.
- ❖Electrons in an FEL are not bound to atoms or molecules.
- ❖The "free" electrons traverse a series of alternating magnets, called a "wiggler," and radiate light at wavelengths depending on electrons' energy, wiggler period and magnetic field.

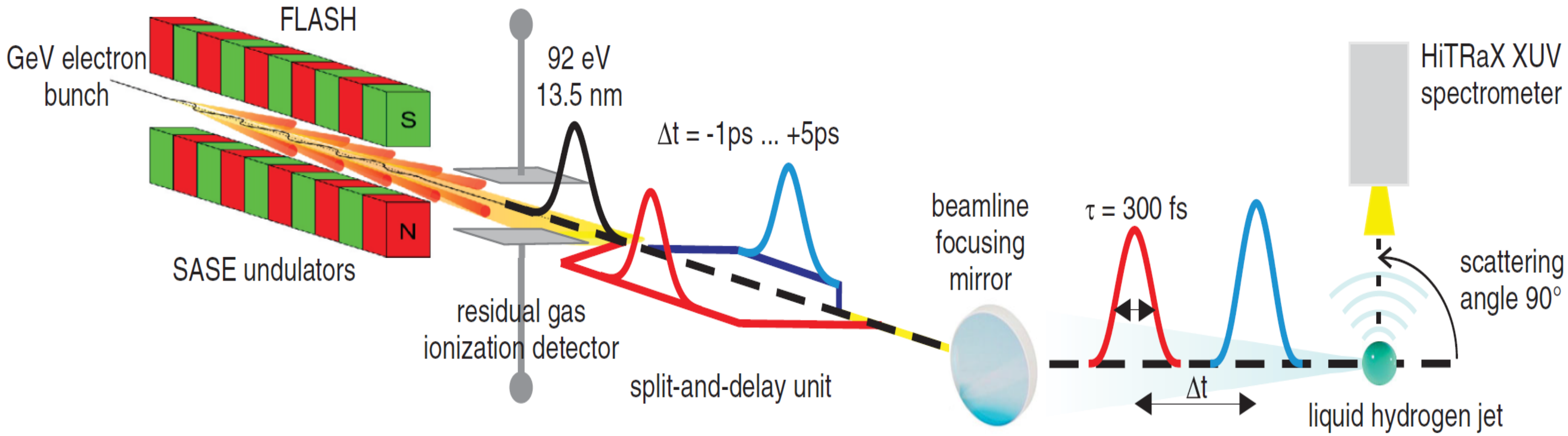


Tremendous XFEL intensity



Fletcher et al, Nature Photonics 2015

Time Delay experiment



U. Zastrau 2014: FLASH(Hamburg)

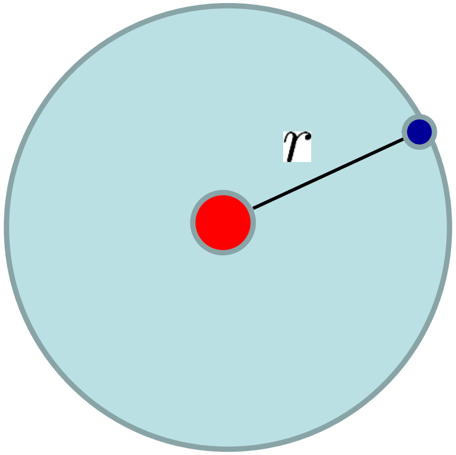
Density Functional Theory

- 1920: Introduction of the Thomas-Fermi model.
- 1964: Hohenberg-Kohn paper proving existence of exact DF.
- 1965: Kohn-Sham scheme introduced.
- 1970 and early 80s: LDA. DFT becomes useful.
- 1985: Incorporation of DFT into molecular dynamics (Car-Parrinello)
- (Now one of PRL's top 10 cited papers).
- 1988: Becke and LYP functionals. DFT useful for some chemistry.
- 1998: Nobel prize awarded to Walter Kohn in chemistry for development of DFT.

Motivation

- Have you solved Schrodinger equation for Hydrogen Atom?

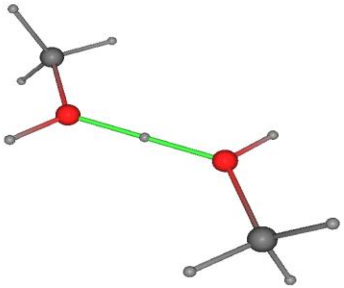
$$H\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$



$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

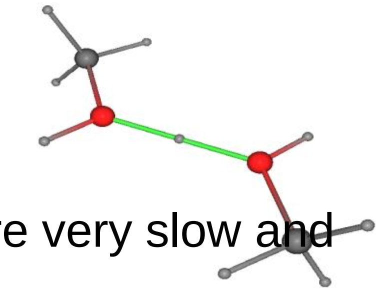
- K.E. P.E.

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$



- Is there an exact solution for complex systems?

Hamiltonian of a molecule



- In a molecule we have many electrons and many nuclei.
- According to **Born-Openheimer** approximations: nuclei are very slow and their kinetic motion are negligible.
- The Hamiltonian should contain
  - The kinetic energy of electrons
  - Potential energy due to electron-electron interactions.
  - Potential energy due to electron-nucleus interactions.

$$H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_{i=1}^{N}\sum_{j\neq i}^{N} \frac{e^2}{4\pi\epsilon_0(r_i - r_j)} - \sum_{i=1}^{N}\sum_{k}^{N_0} \frac{Ze^2}{4\pi\epsilon_0(r_i - r_k)} + V_{\text{ext}}$$

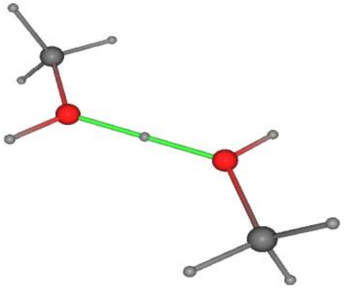
K.E. e-e e-n n-n

- Is there an exact solution for complex systems?

Hohenberg Kohn Theory

- We cannot have two different systems with the same Ground State density.
- The ground state density is a unique function of the nuclei distribution. It is one-to-one relationship.

$$V_{ext} = \sum_{i=1}^{N} \sum_{k}^{N_0} \frac{Z_i Z_k e^2}{4\pi\epsilon_0 (r_i - r_k)}$$



- The electrons will be distributed according to the nuclei distribution.
- The ground state density is related to the minimum energy of the system.

Kohn-Sham Scheme

- The potential energy

$$V_{\mathrm{s}} = V_{ext} + V_{ee}$$

$$V_{\mathrm{s}} = V_{ext}[n(r)] + \int \frac{e^2 n(r) d^3 r}{4\pi\epsilon_0 |r - r'|} + V_{xc}[n(r)]$$

- Schrodinger equation

$$(-\frac{\hbar^2}{2m}\nabla^2 + V_s)\psi(r) = E\psi(r)$$

- The ground state density

$$n(r) = |\psi|^2$$

The ground state is related to minimum energy

- Functional: function of a function

Kohn-Sham Scheme

- Guess an initial density $n(r) = n^{in}(r)$

$$V_s = V_{ext}[n(r)] + \int \frac{e^2 n(r) d^3 r}{4\pi\epsilon_0 |r - r'|} + V_{xc}[n(r)]$$

- Solve Schrodinger equation for ψ and E.

$$(-\frac{\hbar^2}{2m}\nabla^2 + V_s)\psi(r) = E\psi(r)$$

- Calculate the density state   Is it ground state?

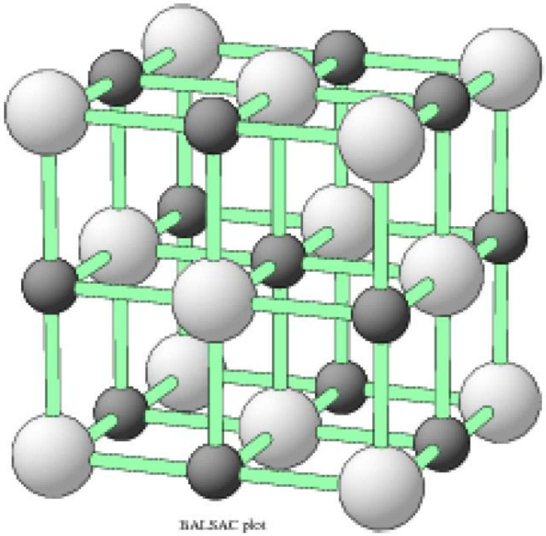
$$n(r) = |\psi|^2$$

The ground state is related to minimum energy

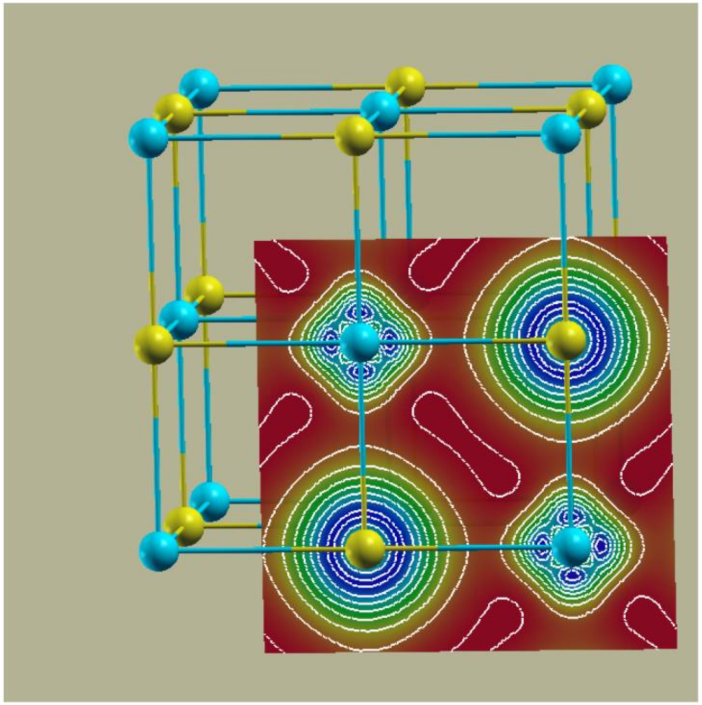
- Functional: function of a function

Wien2K software

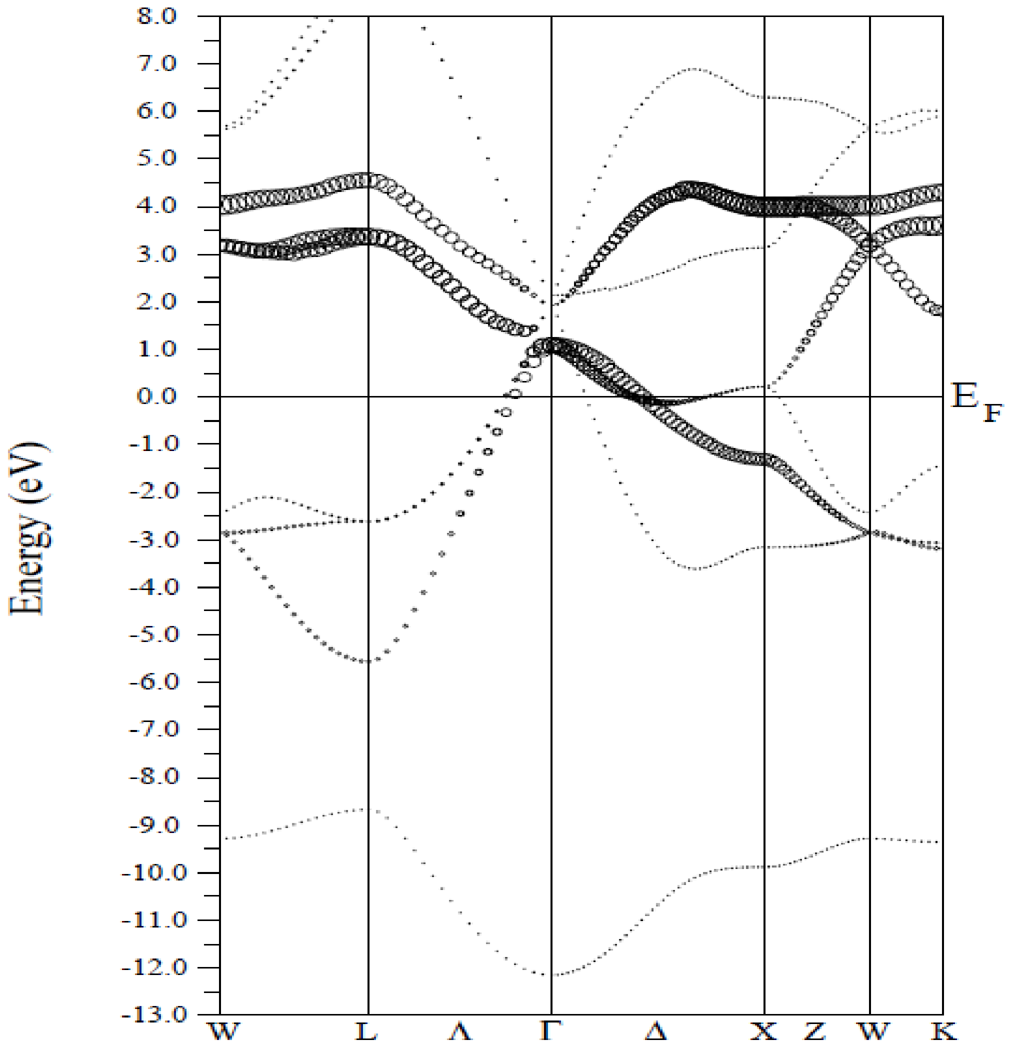
- **TiC in the sodium chloride structure**



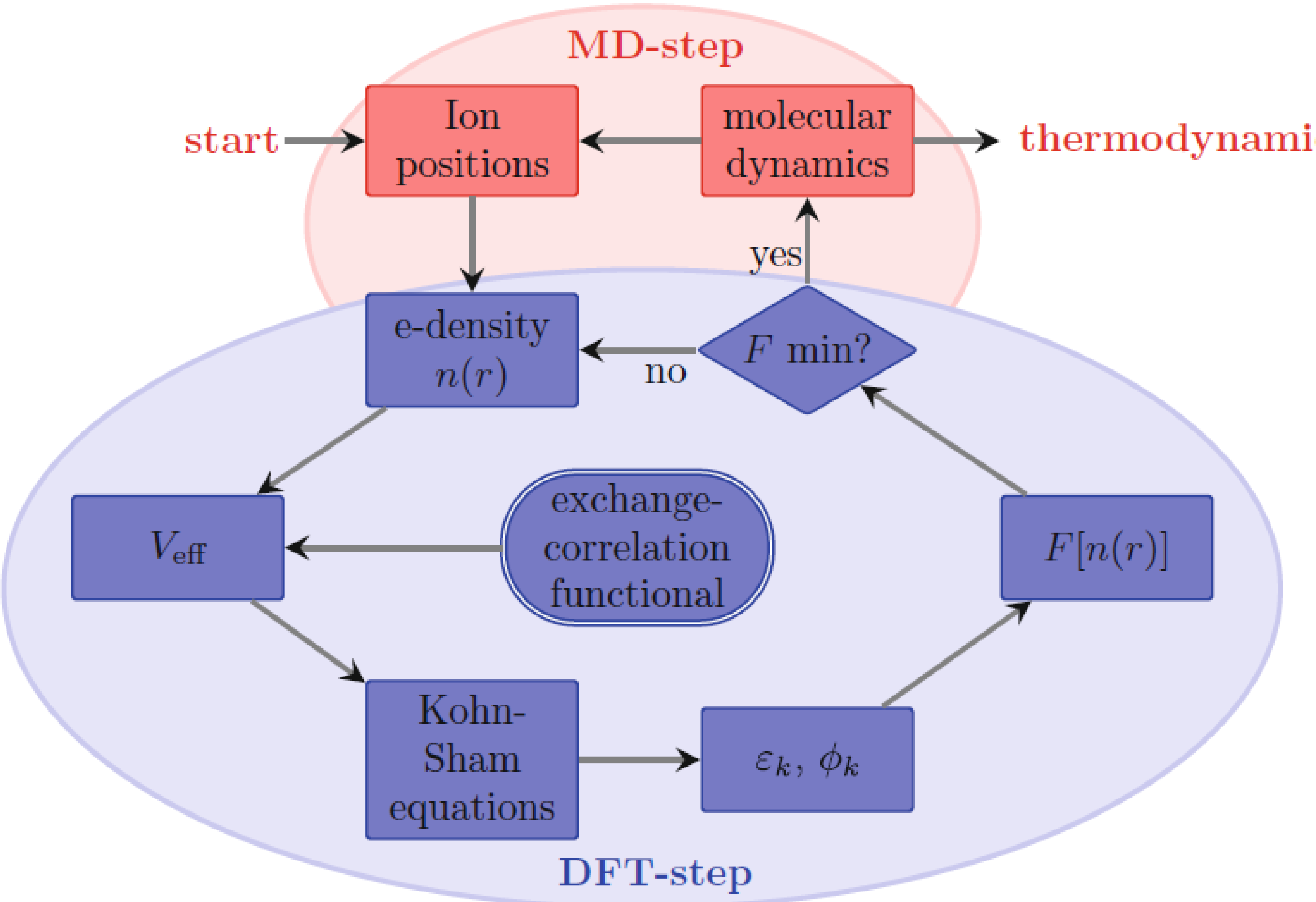
- **The electron density of TiC in (110)**



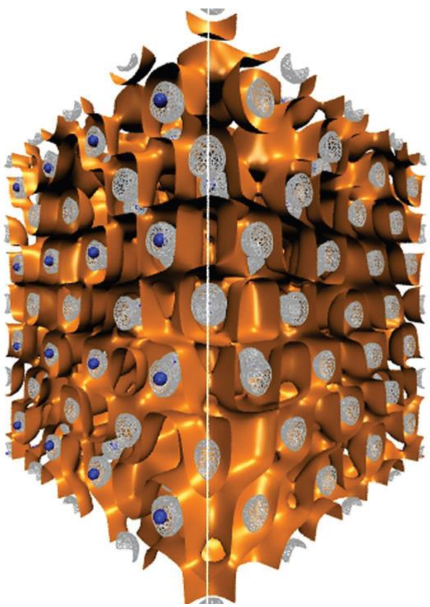
Wien2K software



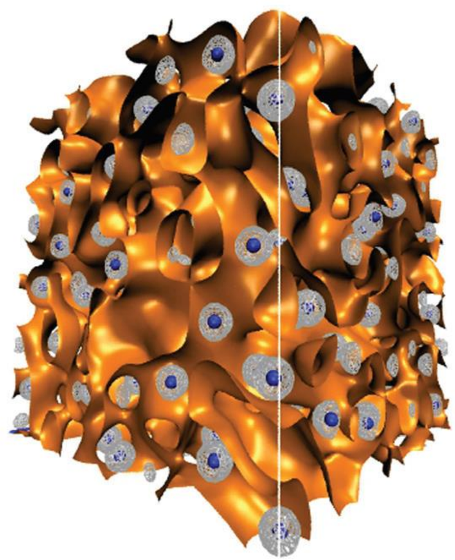
DFT-MD


MD-step
start
Ion positions
molecular dynamics
thermodynami
yes
e-density $n(r)$
F min?
no
V_{eff}
exchange-correlation functional
$F[n(r)]$
Kohn-Sham equations
$\varepsilon_k,\ \phi_k$
DFT-step

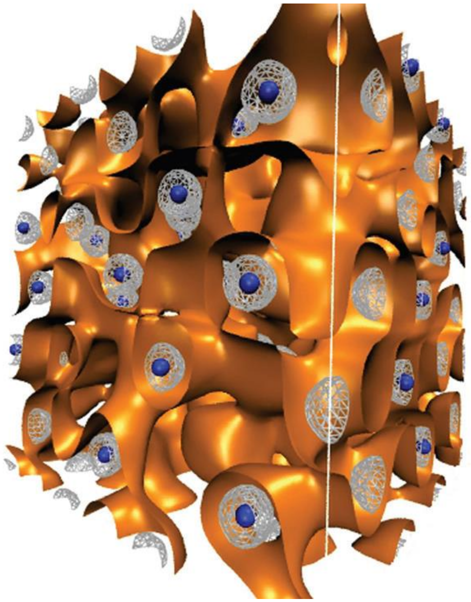
DFT-MD



Solid Aluminum



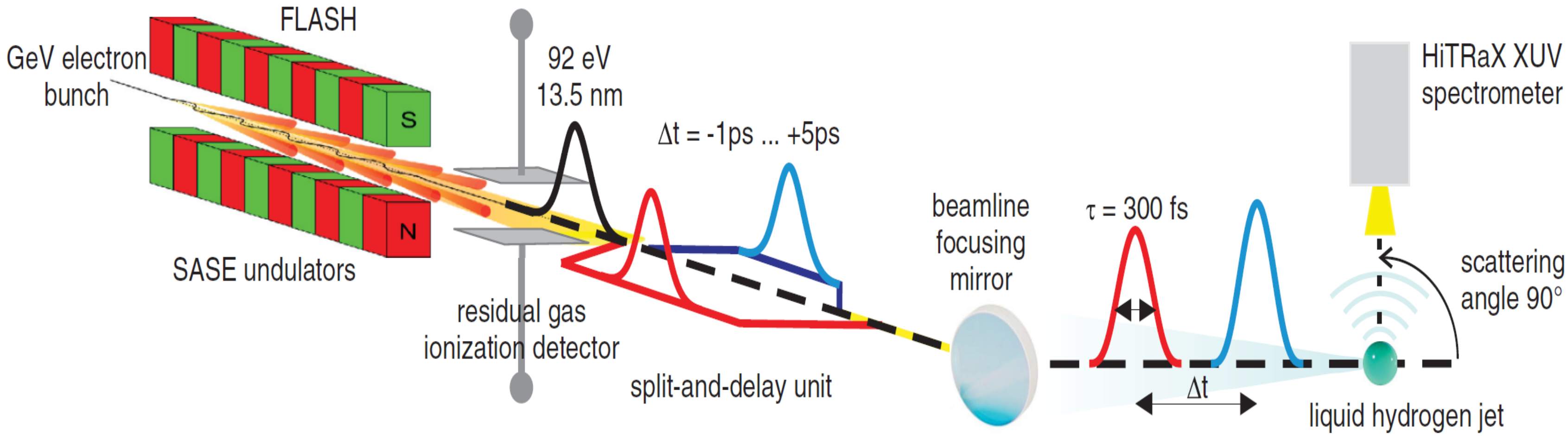
Melting Phase



WDM

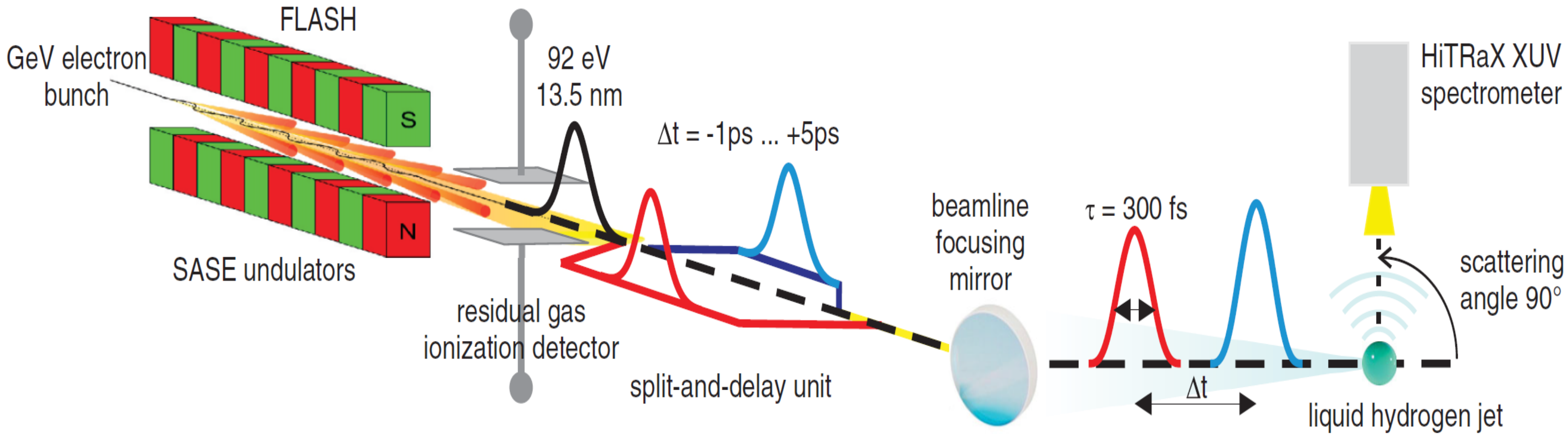
Thanks!

Time Delay experiment



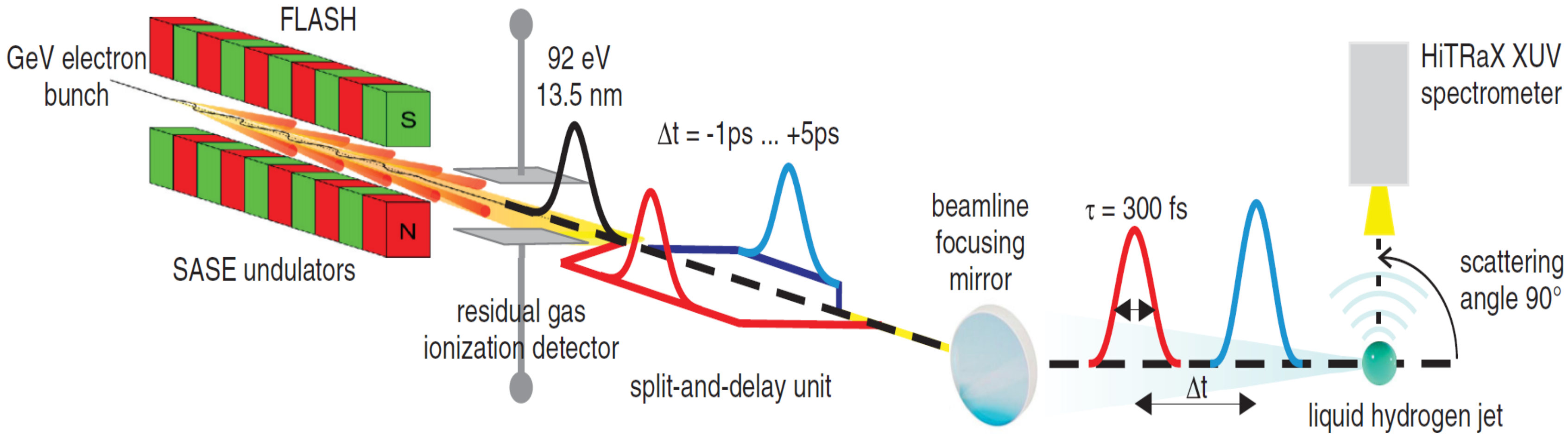
U. Zastrau 2014: FLASH(Hamburg)

Time Delay experiment



U. Zastrau 2014: FLASH(Hamburg)

Time Delay experiment



U. Zastrau 2014: FLASH(Hamburg)