The Abdus Salam
International Centre
for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2369-17

CIMPA/ICTP Geometric Structures and Theory of Control

1 - 12 October 2012

Warm dense matter physics II

Hitoki Yoneda
Institute for Laser Science
Tokyo
Japan

Strada Costiera, 11 - 34151 - Trieste - Italy • Tel. +39 0402240111 • Fax. +39 040224163 • sci_info@ictp.it • www.ictp.it
ICTP is governed by UNESCO, IAEA, and Italy, and it is a UNESCO Category 1 Institute

Warm dense matter physics II

Hitoki Yoneda
Institute for Laser Science

Thanks to
Richard M. More (LBNL)
Hikaru Kitamura (Kyoto U.)

II. Detailed physical model for warm dense matter

Models:

1. from strongly coupled plasma side
2. QMD method
3. Two fluid behavior (EOS)
4. Conductivity
5. Viscosity and diffusion constant

Model of one component plasma

M.S.Murillo, POP, Vol.11-5, p.2964 (2004)

One component plasma

$$-\varepsilon_0 \nabla^2 \phi(r) = Qn(r) - Qn$$ Poisson equation

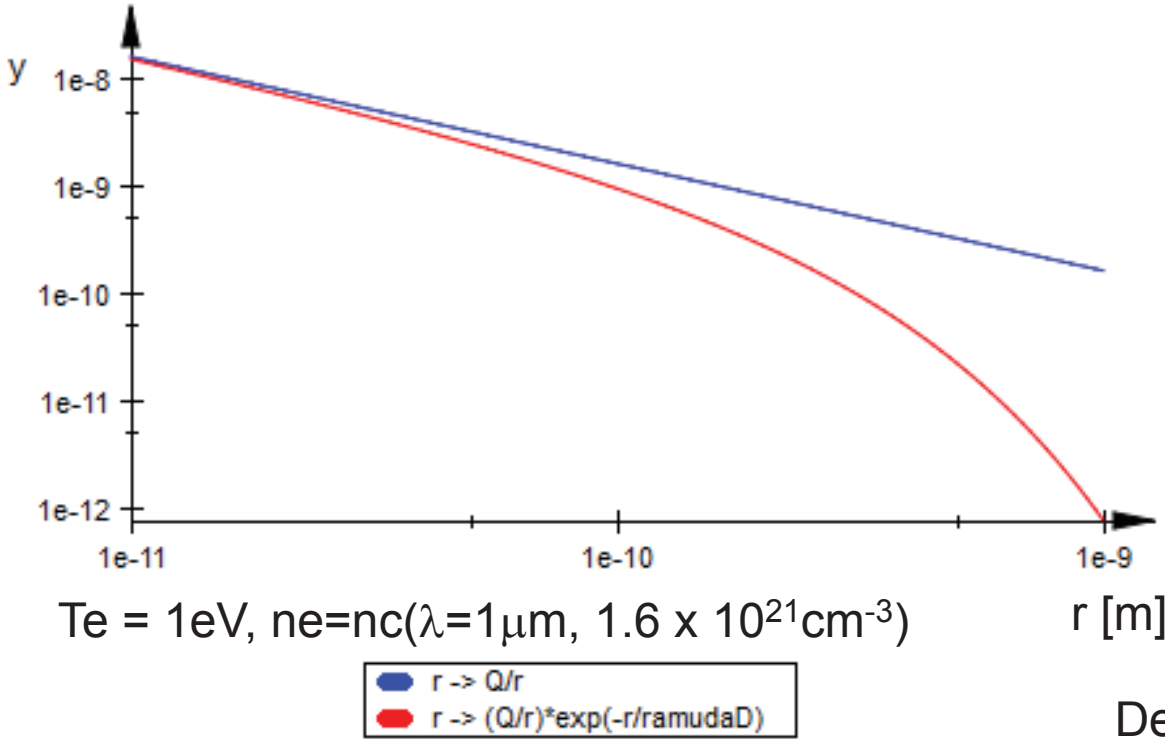
$$n(r) = n \cdot exp\left(-\frac{Q\phi(r)}{T}\right) \approx n\left(1 - \frac{Q\phi(r)}{T}\right)$$ Boltzmann law

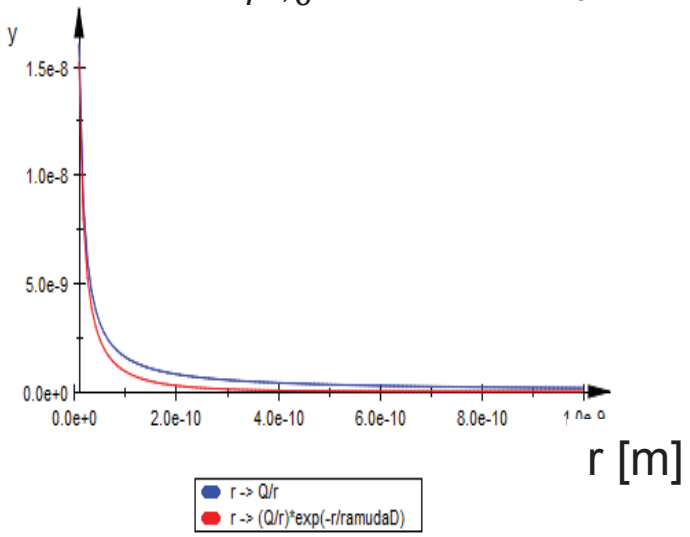
$\frac{Q\phi(r)}{T} << 1$

$$\phi(r) = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r}$$

$$\lim_{r\to 0} r\phi(r) = \frac{Q}{4\pi\varepsilon_0}$$

$$\phi(r) = \frac{Q}{4\pi\varepsilon_0 r} exp\left(-\frac{r}{\lambda_D}\right) \quad (\lambda_D = \sqrt{\varepsilon_0 T / Q^2 n})$$





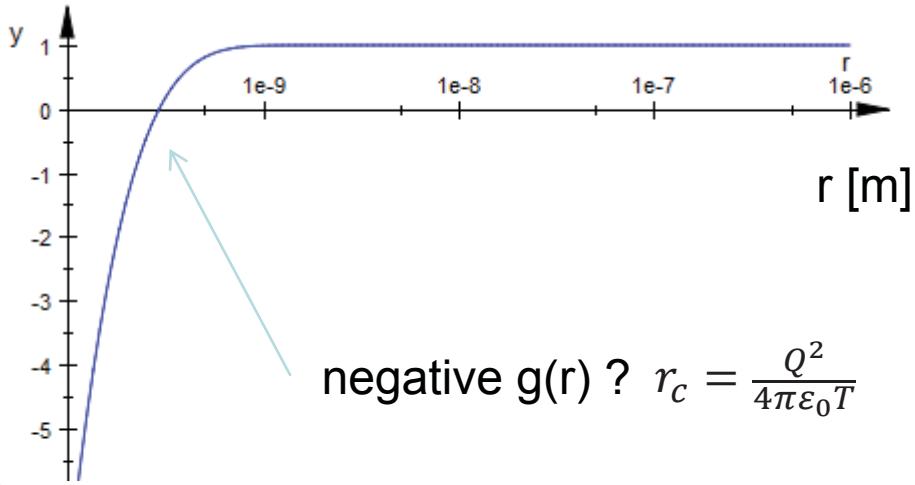
Te = 1eV, ne=nc(λ=1μm, 1.6 x 10^{21}cm^{-3})

Debye-Huckel model

Debye shielding

Distribution function

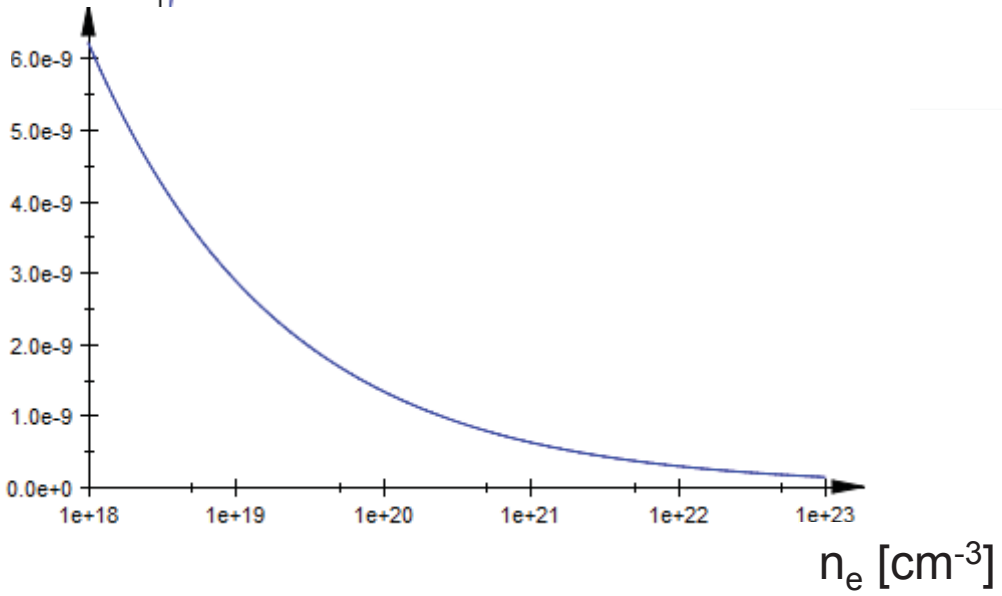
$$g(r) = \frac{n(r)}{n} = \left[1 - \frac{Q^2}{4\pi\varepsilon_0 T r} exp\left(-\frac{r}{\lambda_D}\right)\right]$$



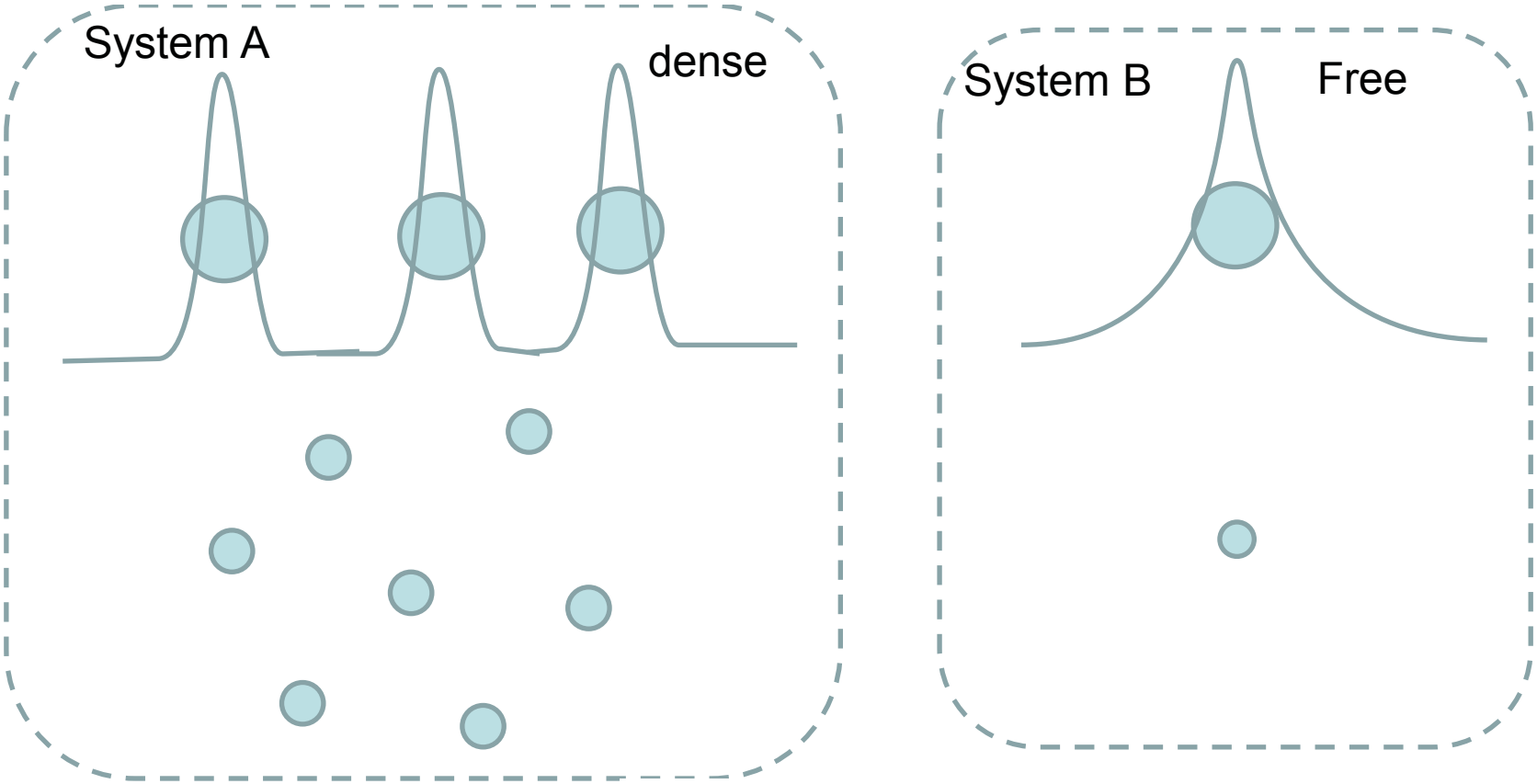
negative g(r) ? $r_c = \frac{Q^2}{4\pi\varepsilon_0 T}$

Radius of ion sphere

$$a = (3/4\pi n)^{1/3}$$



$r_c \ll a$



Potential energy Ea - Eb

In the D-H model, $\lim_{r\to 0}\left[\phi(r) - {}^{Q}/_{4\pi\varepsilon_0 r}\right] = -\frac{Q}{4\pi\varepsilon_0\lambda_D}$ $\phi(r) = \frac{Q}{4\pi\varepsilon_0 r}exp\left(-\frac{r}{\lambda_D}\right)$

Potential energy $= -\frac{Q^2}{4\pi\varepsilon_0\lambda_D}\times\frac{N}{2}$

$$\text{Total energy} = \frac{3}{2}NT - \frac{N}{2}\frac{Q^2}{4\pi\varepsilon_0\lambda_D} = NT\left(\frac{3}{2} - \frac{\sqrt{3}}{2}\Gamma^{3/2}\right)$$

$$\text{Pressure} = nT\left(1 - \frac{\sqrt{3}}{6}\Gamma^{3/2}\right)$$

More precision,

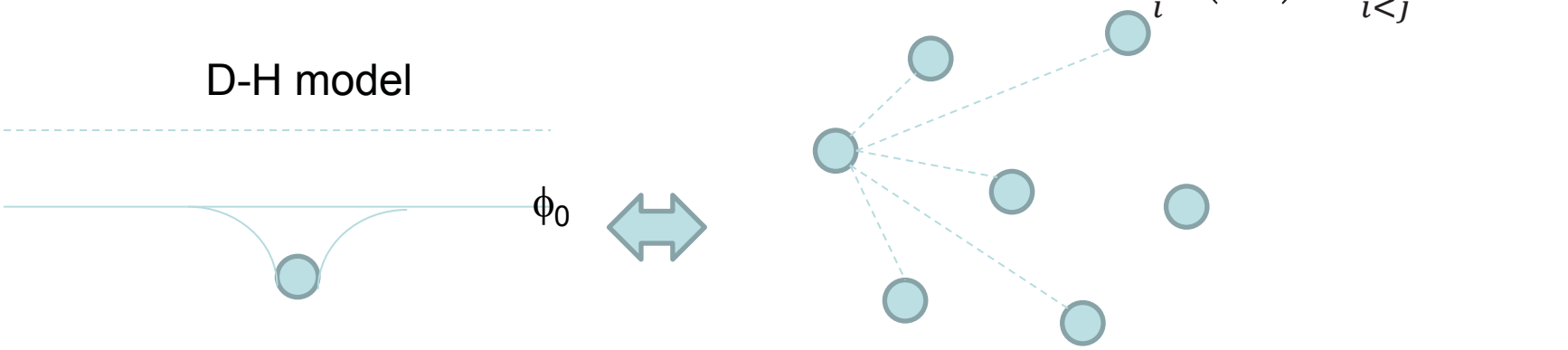
$$Energy = \frac{3}{2}NT + \frac{2\pi N^2}{\Omega}\int_0^\infty drr^2(g(r)-1)\frac{Q^2}{r}$$

$$Pressure = NT - \frac{2\pi n^2}{3}\int_0^\infty drr^3(g(r)-1)\frac{d\ Q^2}{dr\ r}$$

$$g(r) = \frac{1}{nN}\left\langle \sum_{i<j}^{N} \delta(\mathbf{r}-(\mathbf{r}_i-\mathbf{r}_j))\right\rangle \qquad \langle F\rangle \equiv \frac{\int drF\cdot\exp(-H/T)}{\int dr\ \exp(-H/T)}$$

$$H = \sum_i \left(\frac{p^2{}_i}{2m}\right) + \sum_{i<j} U_{ij}(r_{ij})$$

D-H model



Multi particle interaction -- very difficult to solve

MD, MC, ….

From DFT theory,

$$g(r) = exp\left(-\frac{Q^2}{rT} + h(r) - c(r) + B(r)\right)$$

Pair correlation function

Direct correlation function

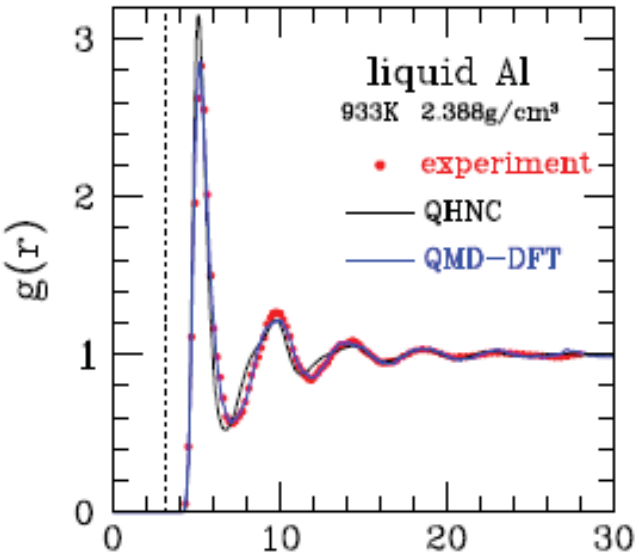
Bridge function

Ornstein Zernike equation

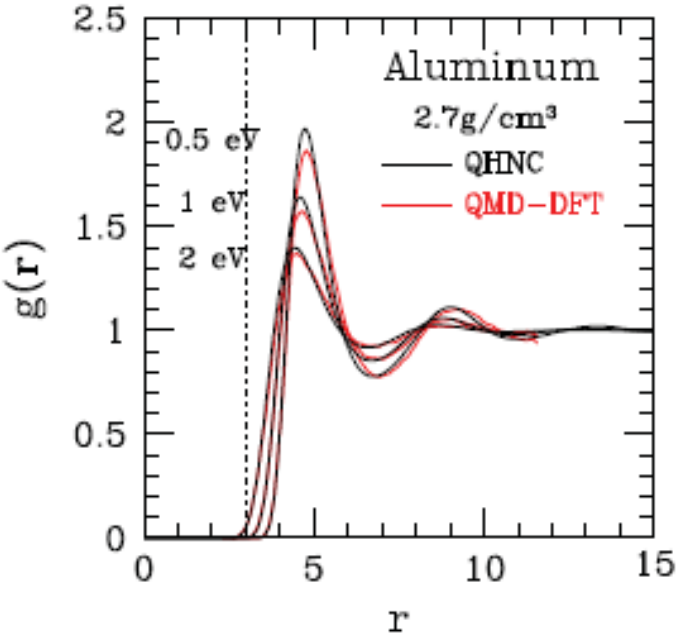
$$h(r) = c(r) + n\int d^3r' c(r')h(r - r')$$

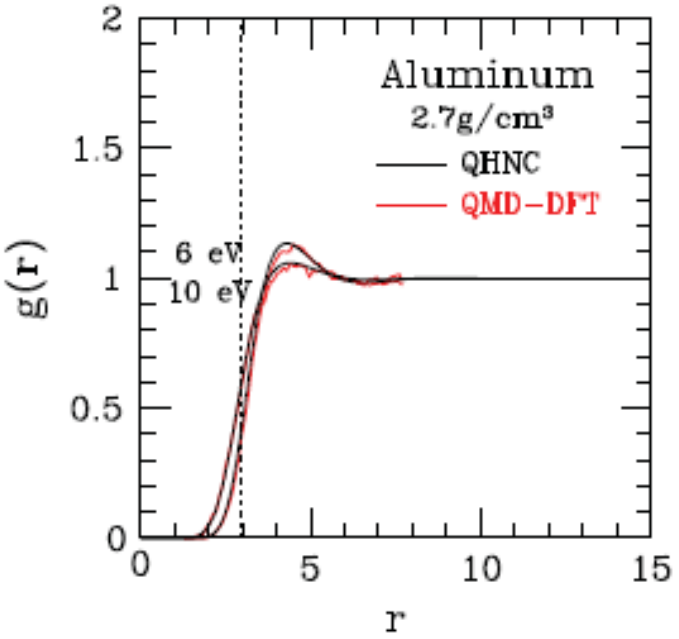
Radial distribution function

D. Saumon, et al., High Energy Density Physics 8 (2012) 150~153



Friedel oscillation decreases when temperature increas





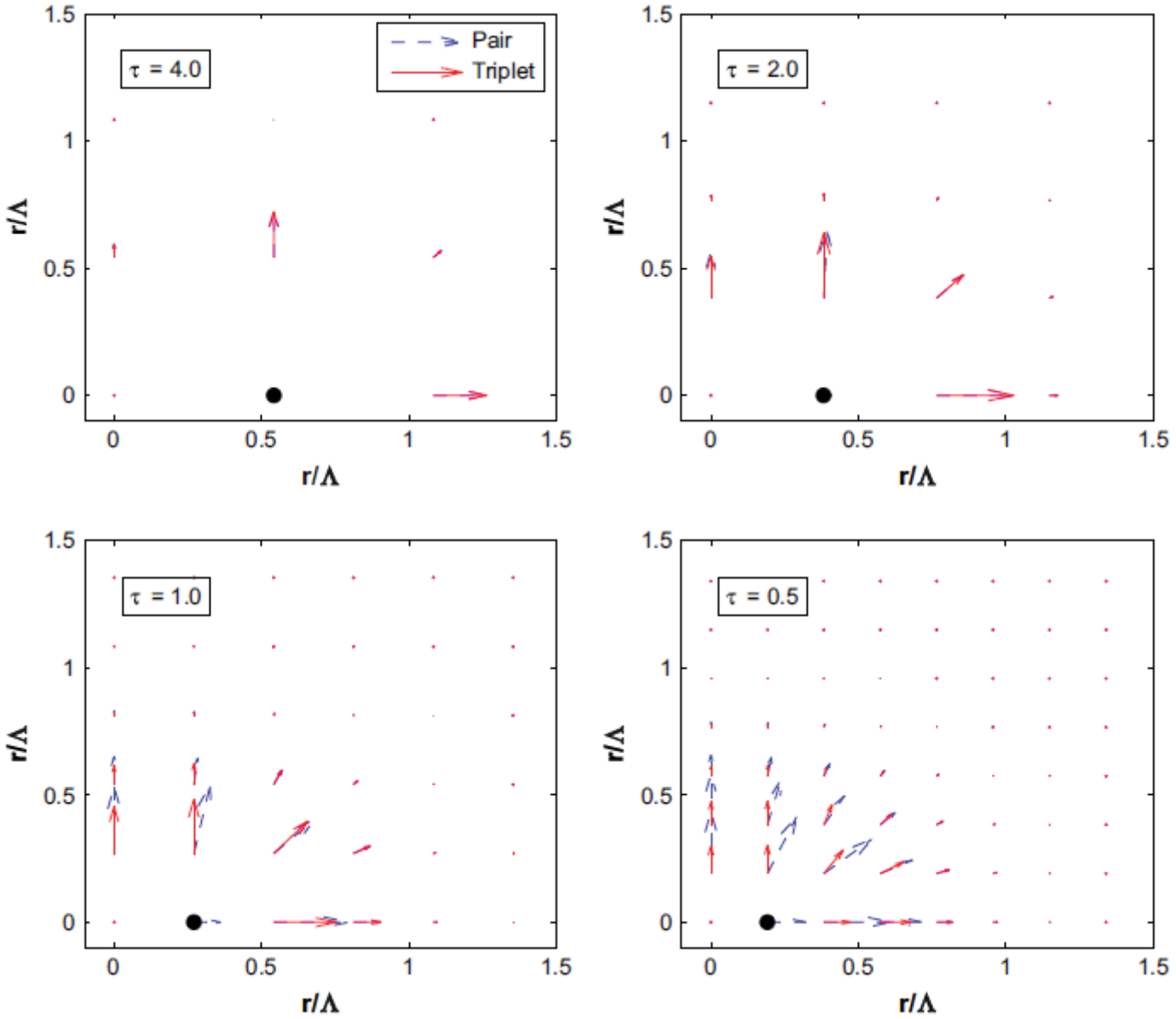


Fig. 1. **Two-body (solid arrows) and three-body (dashed arrows) forces**, determined by the potentials (36) and (37), are plotted at t . 4.0, 2.0, 1.0 and 0.5 in the top left, top right, bottom left and bottom right panels, respectively. The force is due to a pair of particles located at a/2 on the abscissa, with the particle at ta/2 indicated by a black dot. The force is plotted on a lattice with spacing a/2, while the axes are plotted in units of L. The units of force are 12kBTF/a.

QMD and MD

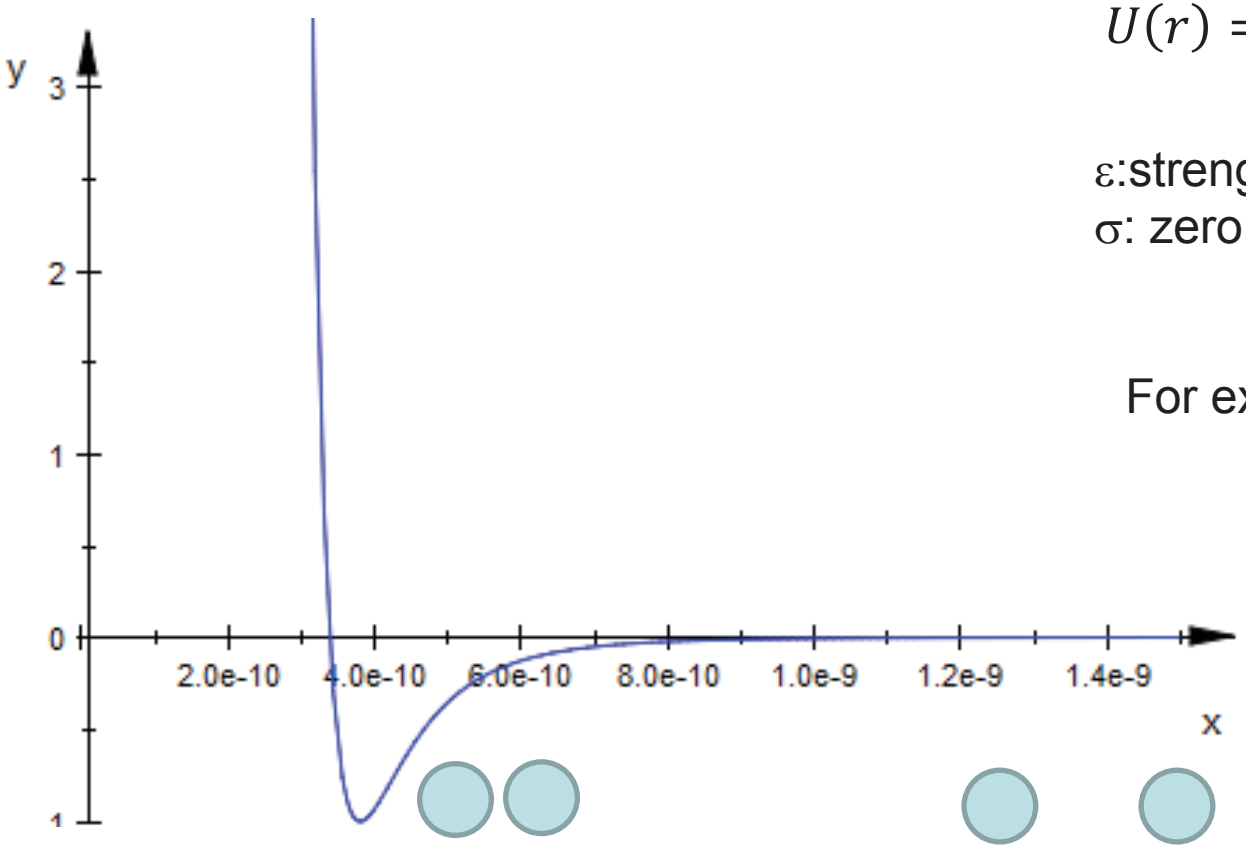
Molecular Dynamic simulation

Lennard-Jones potential

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

ε:strength of potential energy
σ: zero energy radius

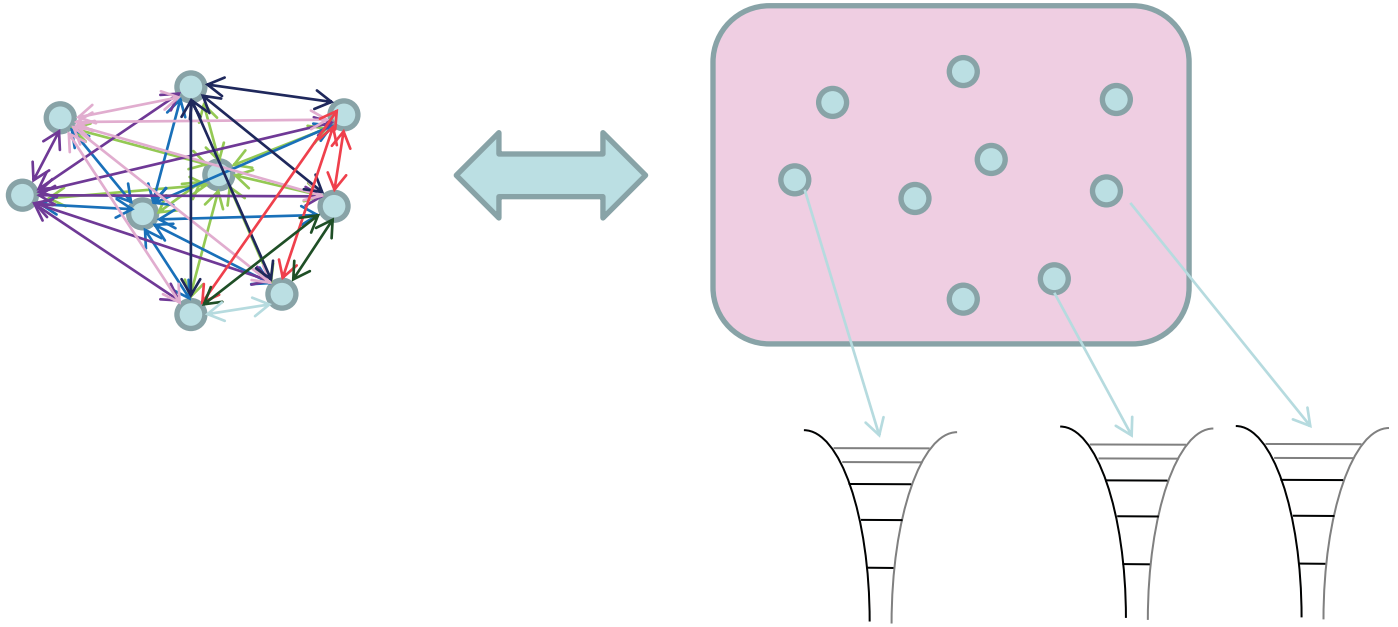
For example: Ar
ε=1.654x10^{-21} J
σ=3.405 x 10^{-10} m



$$F(r) = -\frac{dU(r)}{dr} = 4\varepsilon\frac{\varepsilon}{\sigma}\left[12\left(\frac{\sigma}{r}\right)^{13} - 6\left(\frac{\sigma}{r}\right)^{7}\right]$$

$$PV = NkT - \frac{1}{3}\left\langle\sum_i^N r_i \cdot F_i\right\rangle$$

DFT calculation in solid-state physics:

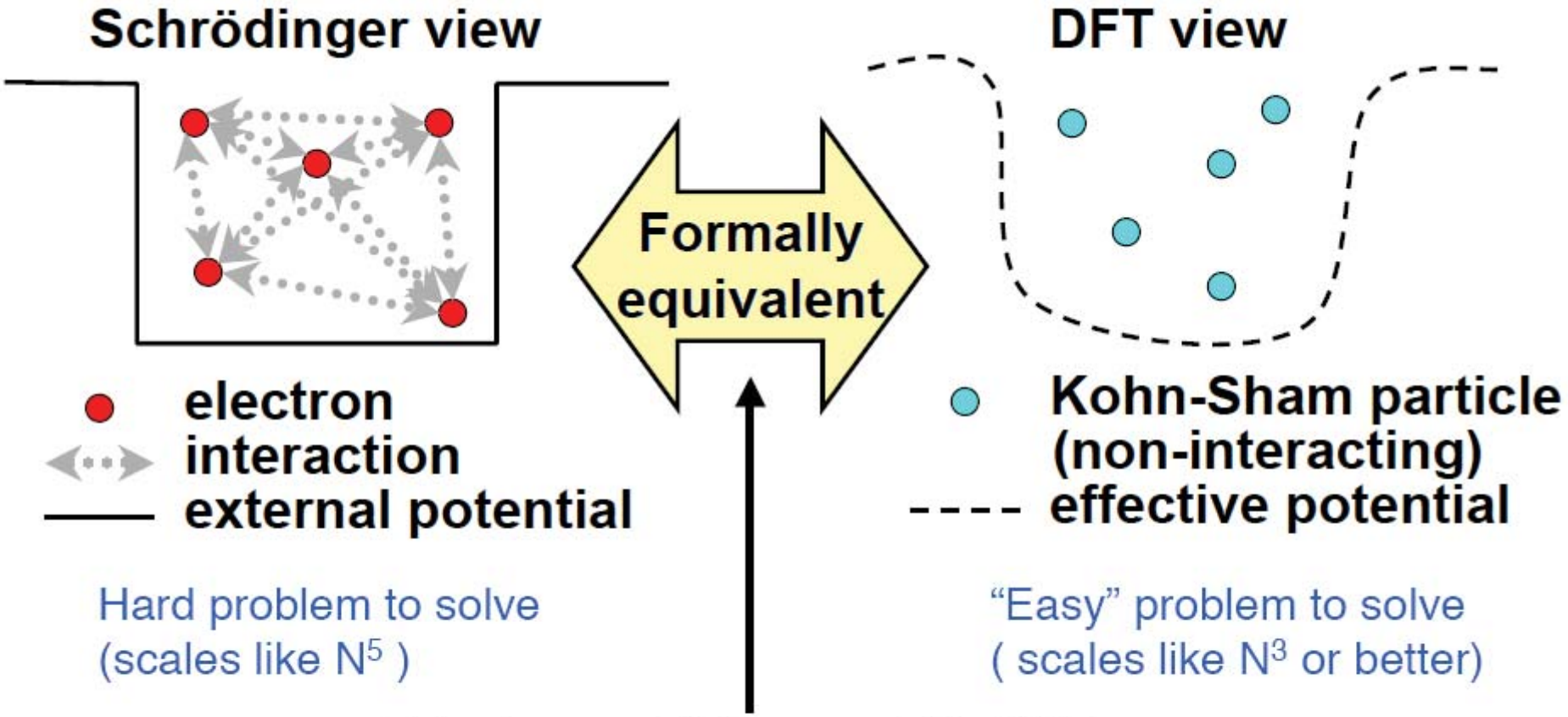


Use known wave function of each atom

~~Excitation state~~

Modeling

Density Functional Theory



Hohenberg and Kohn proved this (1964)

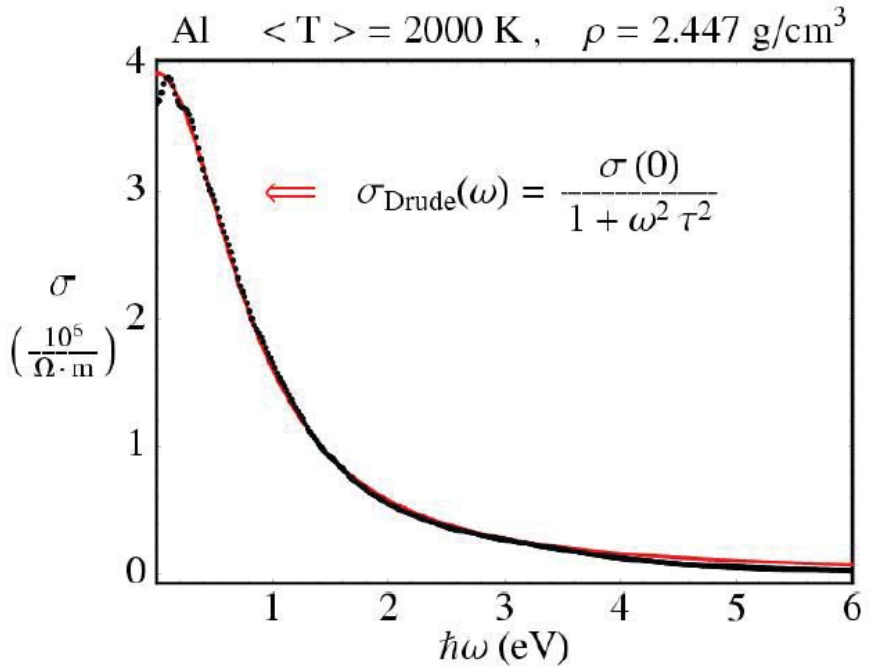
Nobel prize in Chemistry for Kohn in 1998

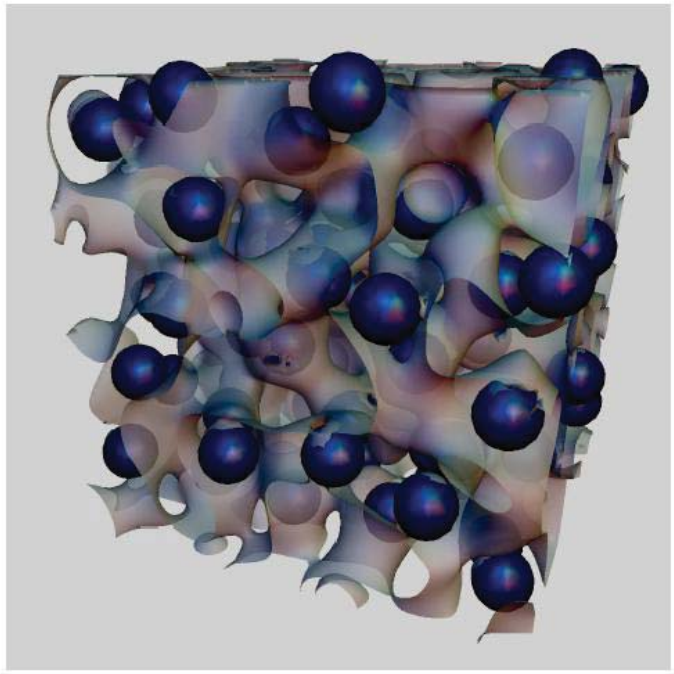
Sandia National Laboratories

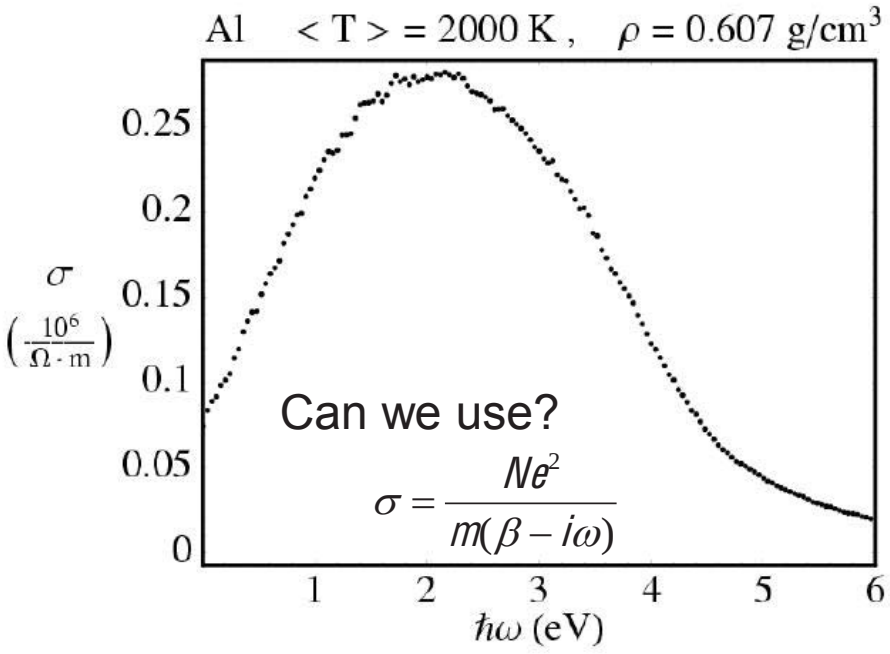
(1) P.Hohenberg and W.Kohn: Inhomogeneous electron gas,Phys.Rev.136,B864(1964).
(2) W.Kohn and L.J.Sham: Self-consistent equations including exchange and correlation effects,Phys.Rev.140,A 1133 (1965).

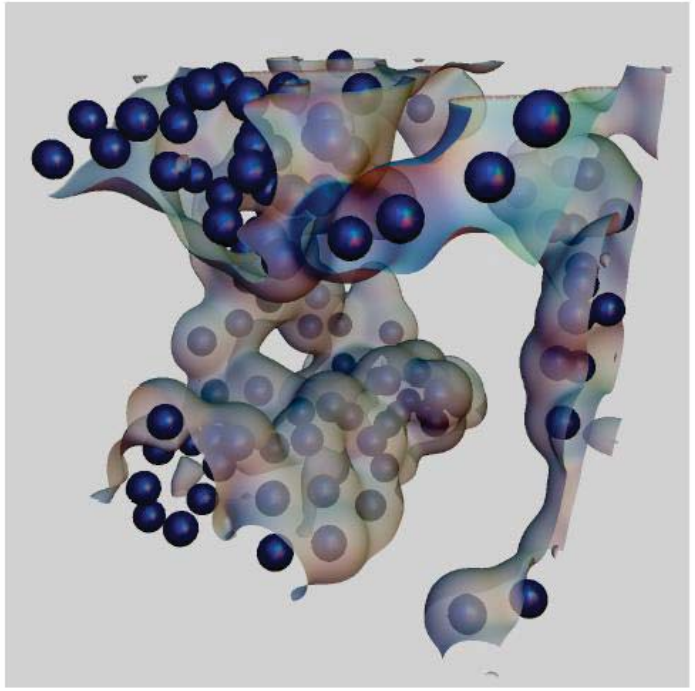
QMD simulation view of wdm Al interia.

Michael Desjarlais, 2008 WDM school









Jiayu Dai, Yong Hou, and Jianmin Yuan, PRL 104, 245001 (2010)

Details in electronic state levels

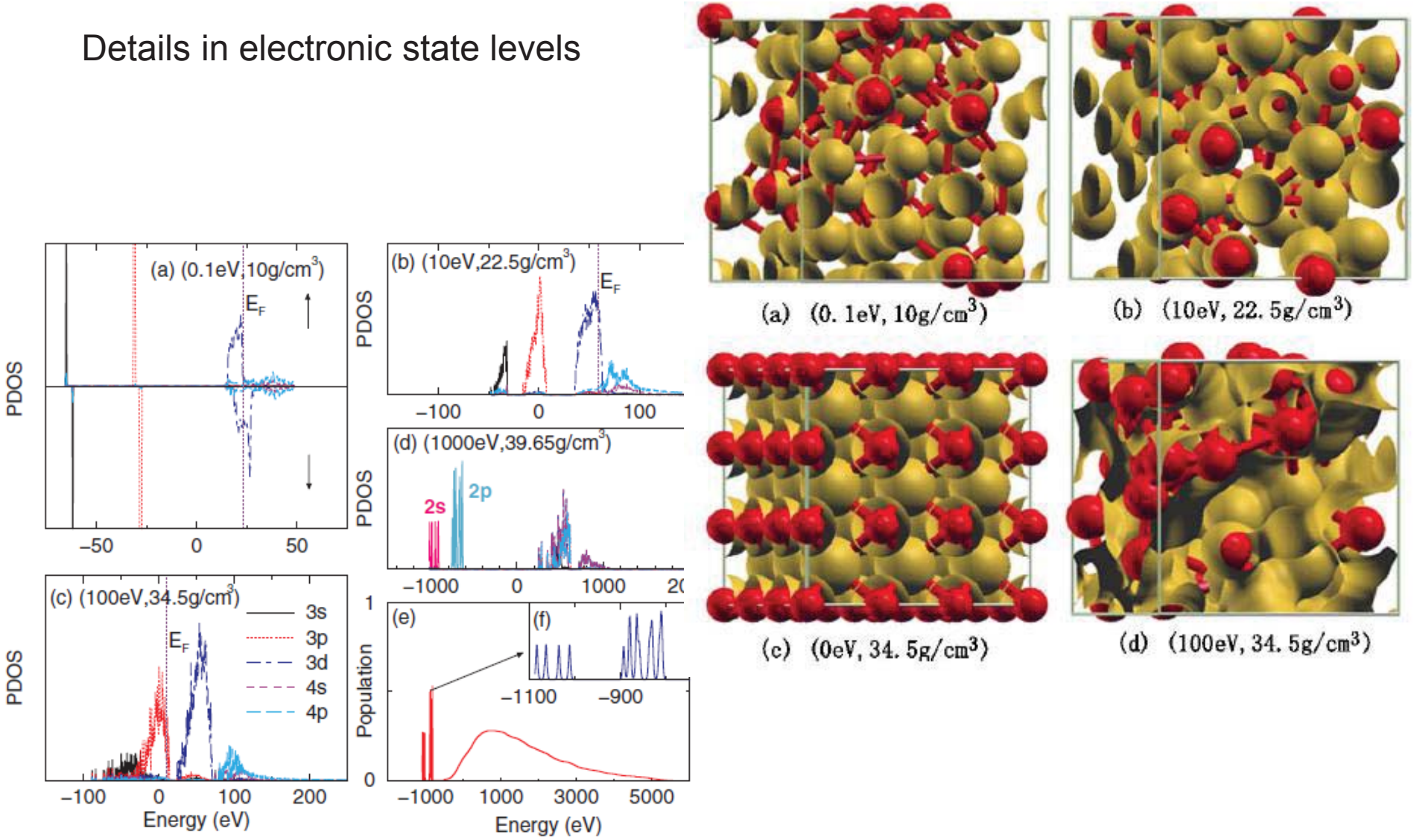
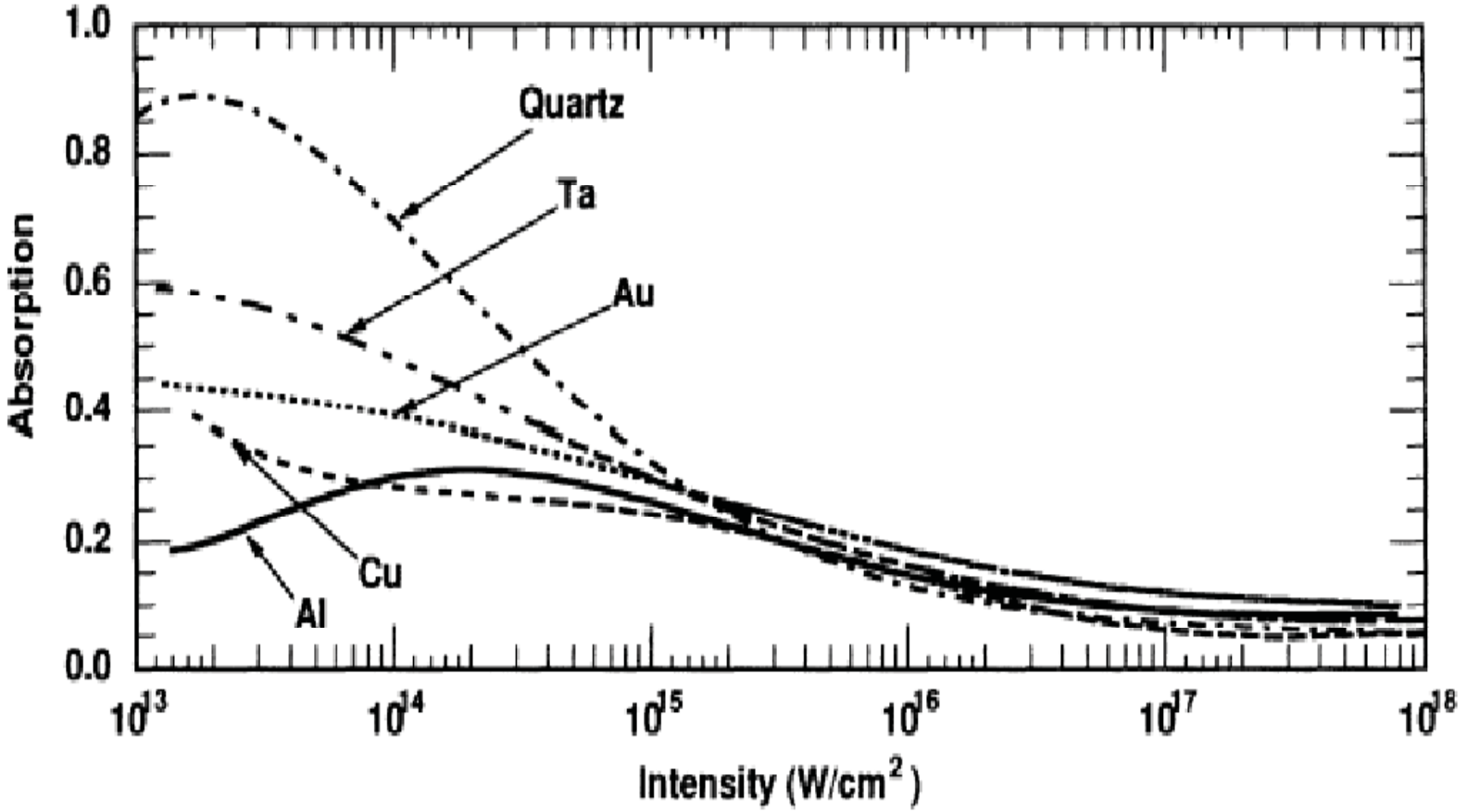


FIG. 3 (color online). (a)–(d) Typical PDOS of different orbitals at different temperature-density points (arbitrary units). The arrows represent spin up and spin down. (e) The electron population distribution at 1000 eV, 39:65 g=cm3; (f) a slice for the electron population for 2s and 2p electrons.

We have measured Au, Cu, Al, W, Mo, Sn, Fe, SS304, SiO_2.

For λ=745nm

various trajectory



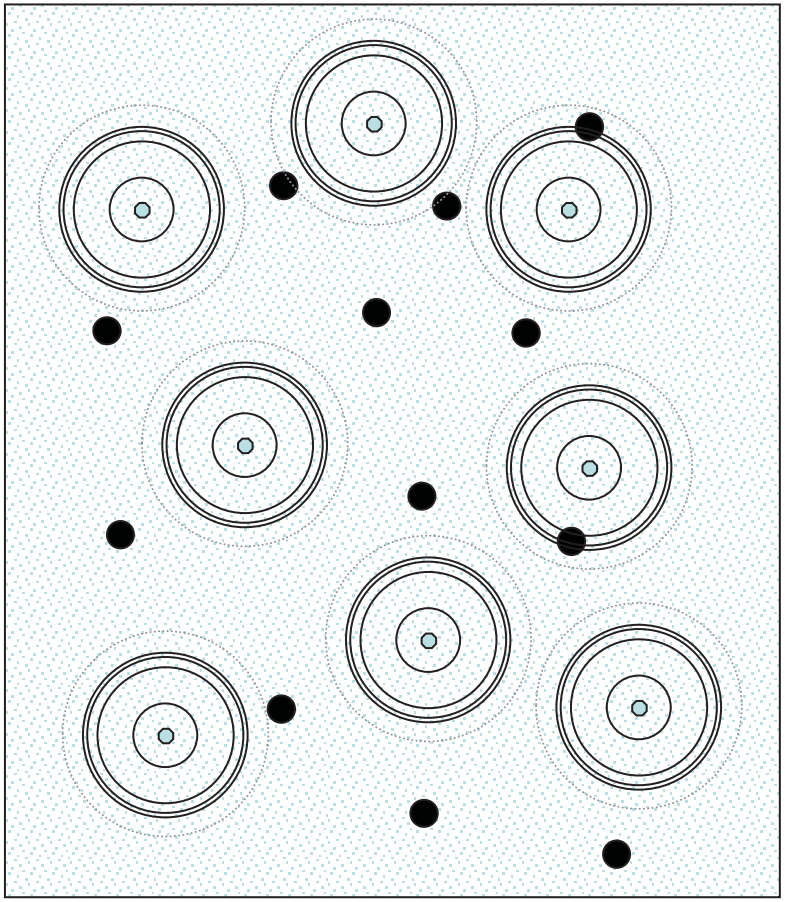
ntinued

0 0.5 1 1.5

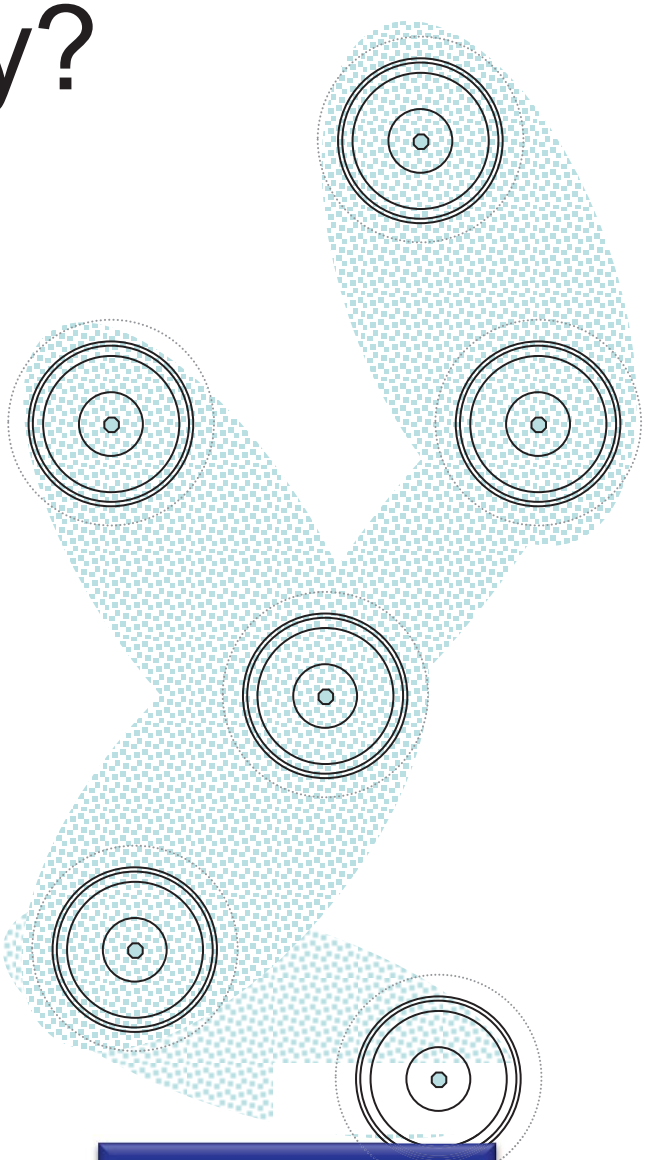
R_p/R_s

Previous experiments(D.F.Price, et al.,PRL, Vol.75-2, 252 (1995))

Which way?



homogeneous
Non-localization

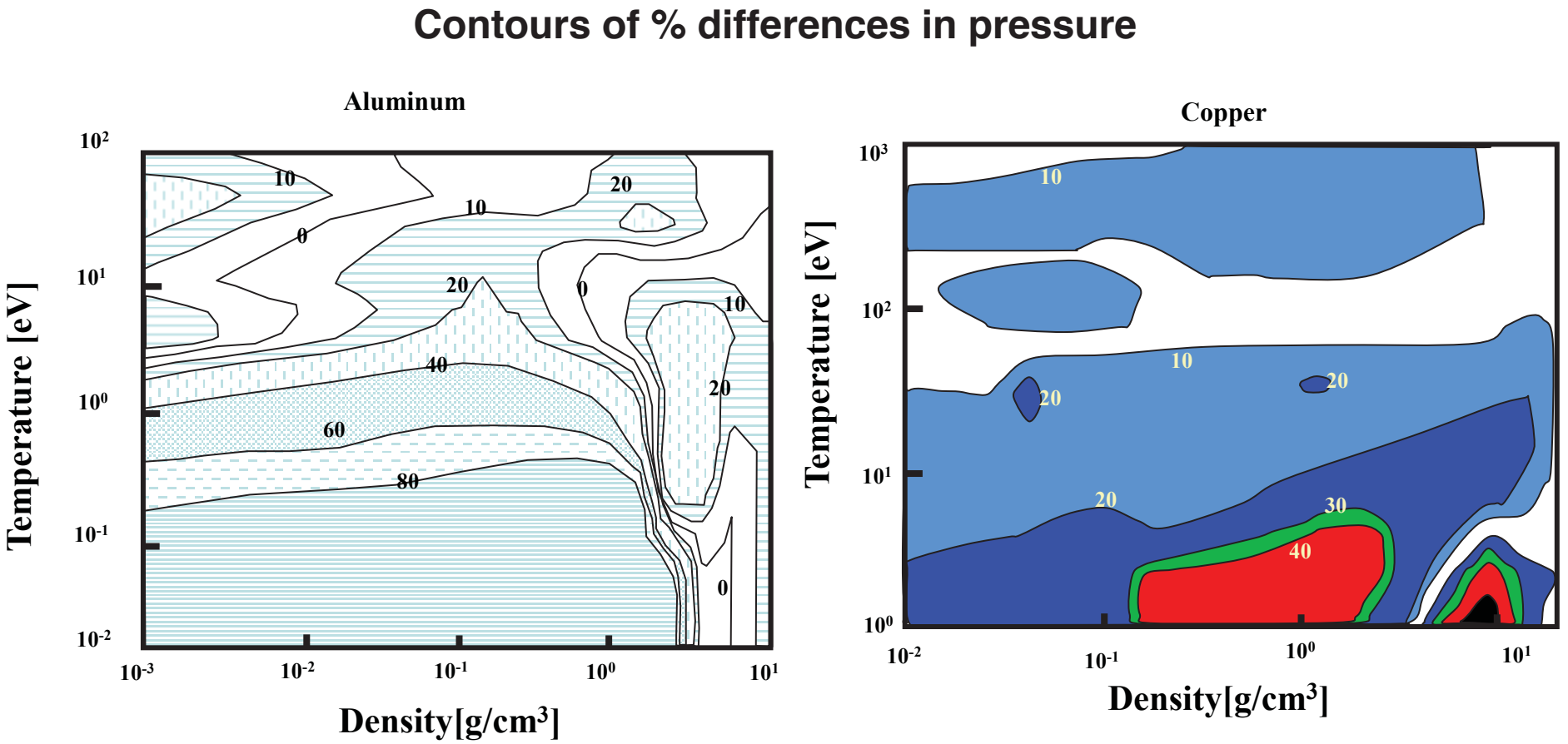


Inhomogeneous
localization

Equation of States

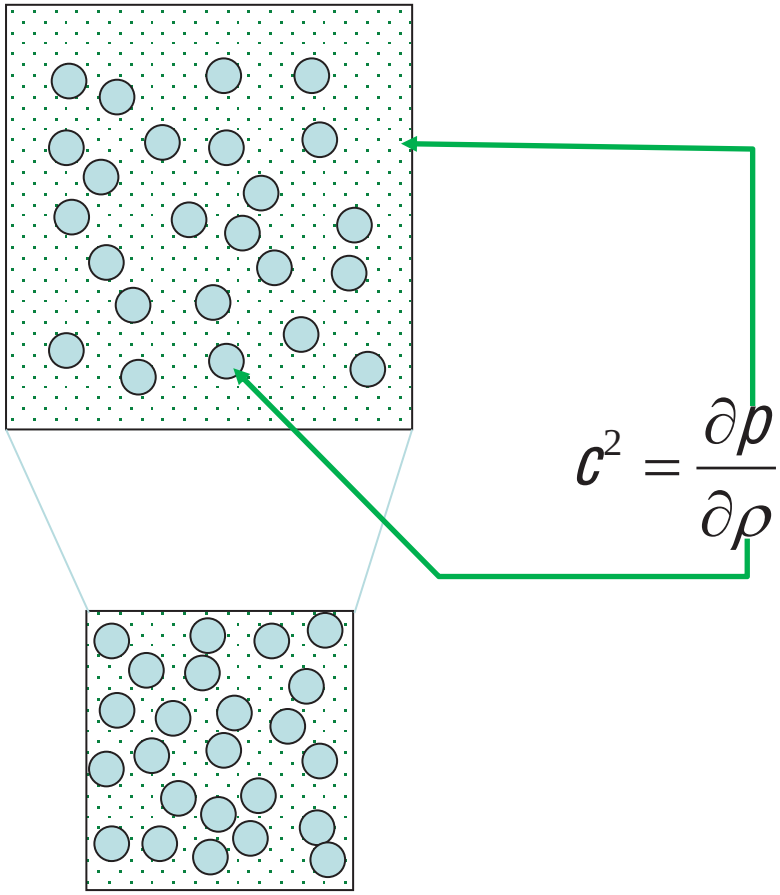
Why WDM physics?

Global Equation of States: lack of data and accuracy in WDM



after R.W.Lee, TESLA Colloquium 2001

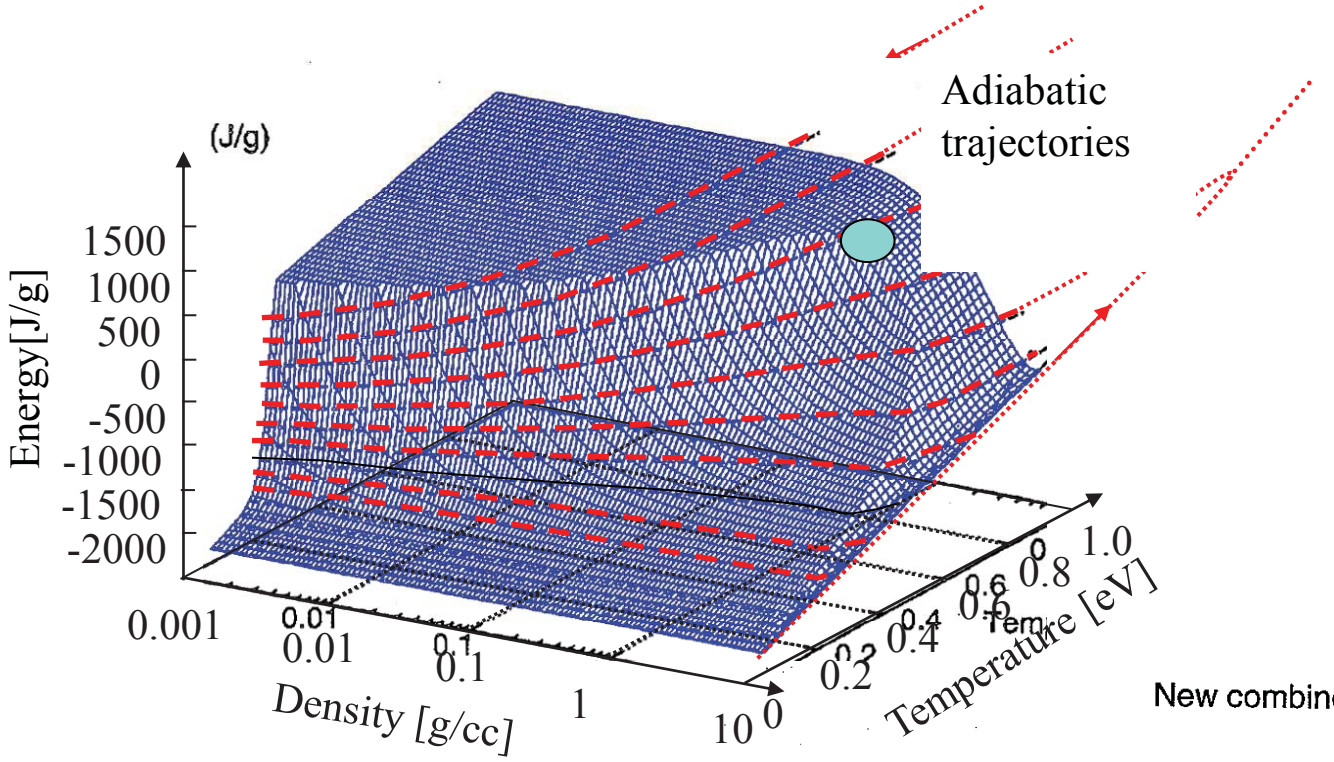
What happen in two fluid region?

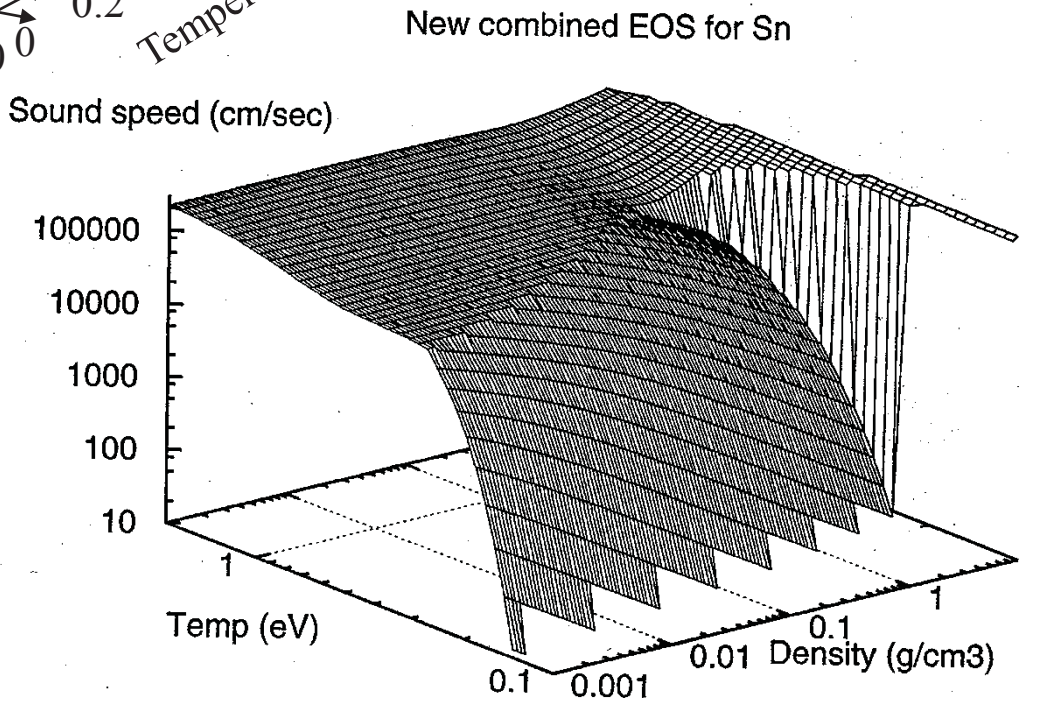


compression

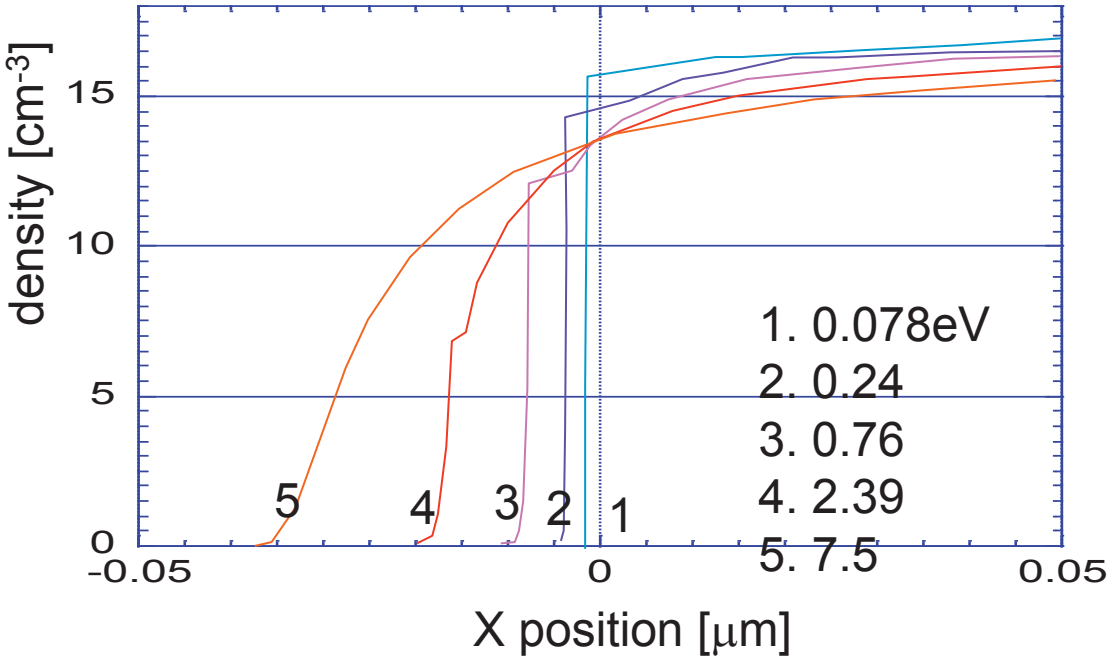
$$c^2 = \frac{\partial p}{\partial \rho}$$

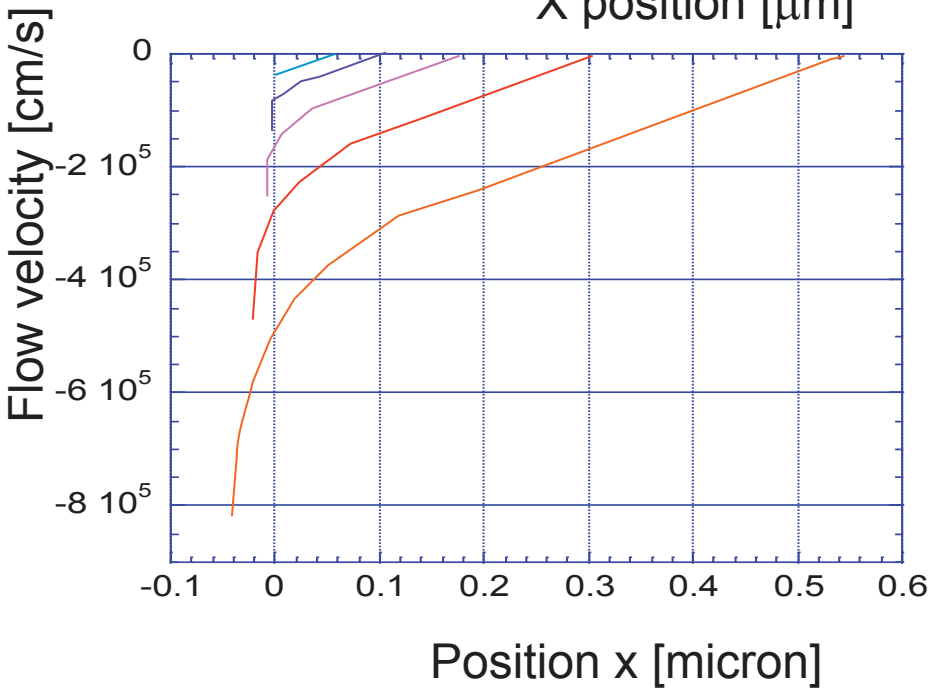
Independent parts contribute different physical parameters.

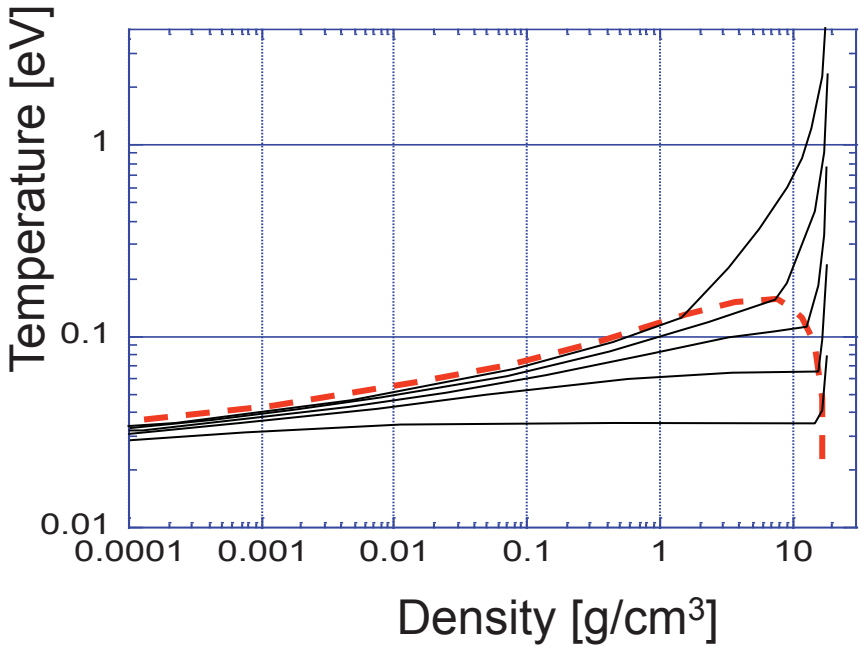

Adiabatic
trajectories
(J/g)
Energy[J/g]
1500
1000
500
0
-500
-1000
-1500
-2000
0.001
0.01
0.1
1
10
Density [g/cc]
0
0.2
0.4
0.6
0.8
1.0
Temperature [eV]


New combined EOS for Sn
Sound speed (cm/sec)
100000
10000
1000
100
10
1
0.1
Temp (eV)
0.001
0.01
0.1
1
Density (g/cm3)

Due to EOS feature, we can expect sharp expansion front with some condition.



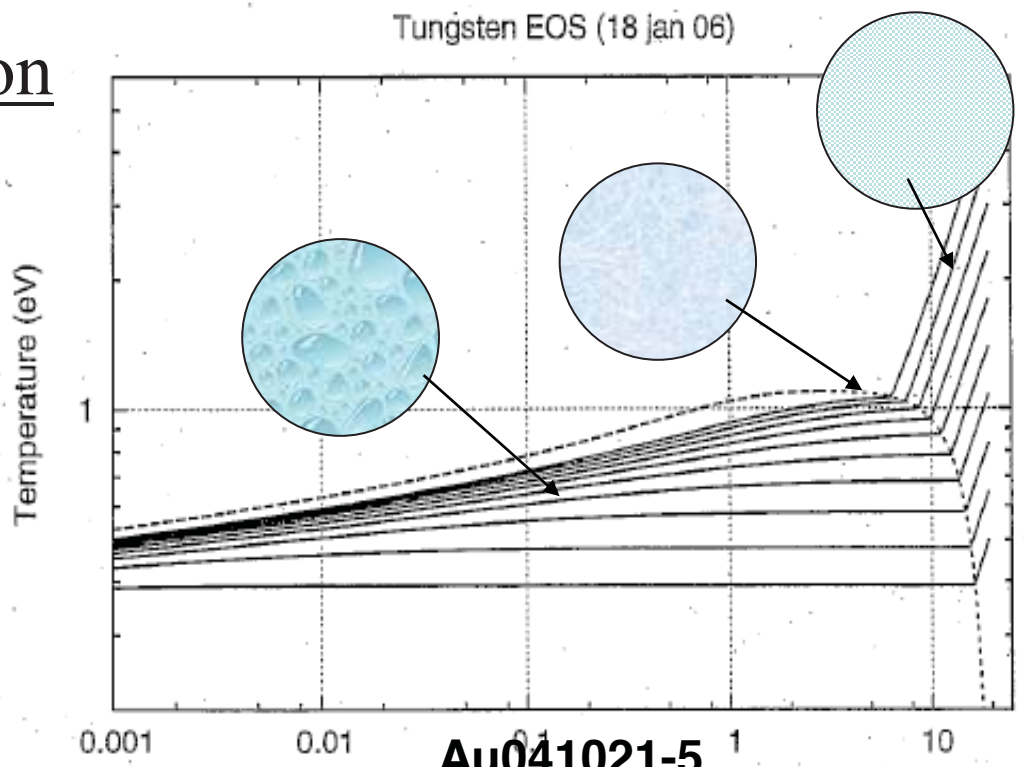


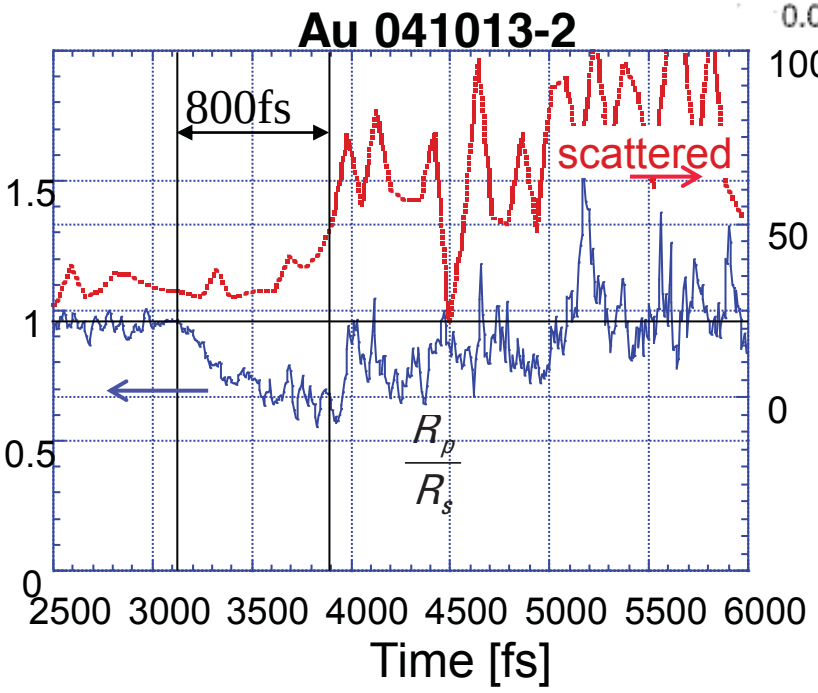


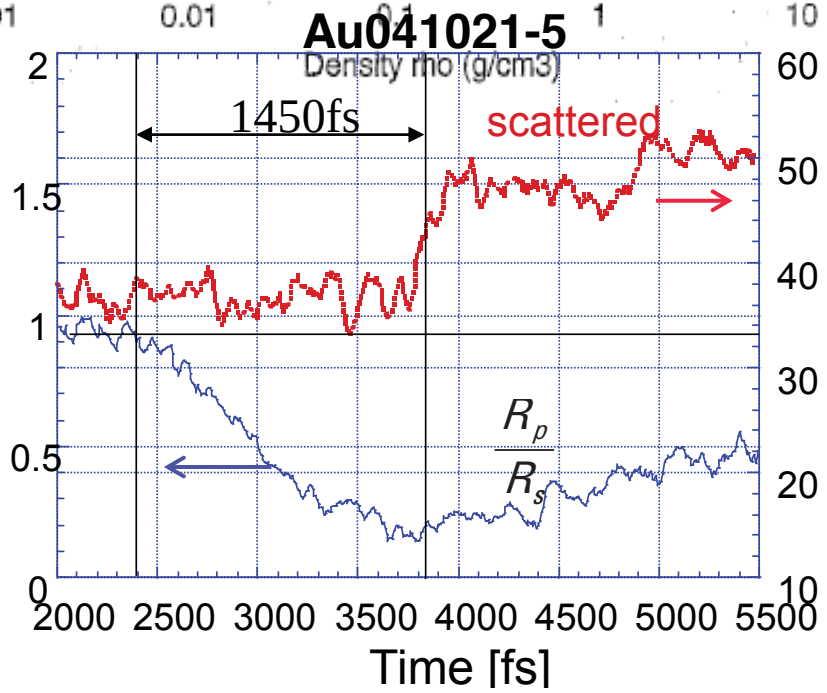
Detection of 2ϕ fluid region diffuse scattering signals

Au 0.6~2.6ps

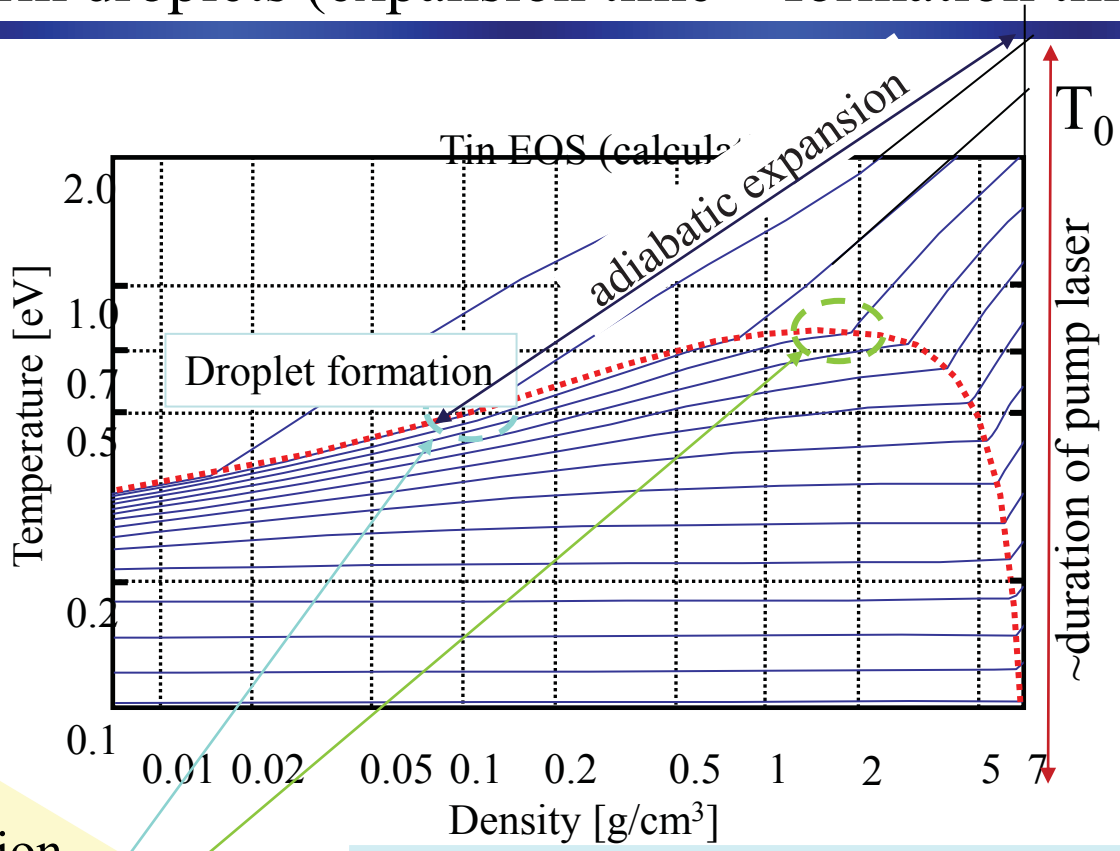
W 0.75~1ps

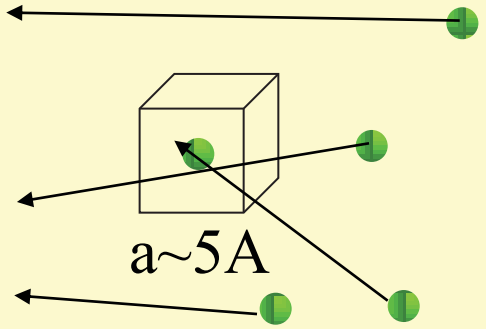






Time required to form droplets (expansion time + formation time)





Rate of droplet formation

$$\frac{1}{R_{droplet}} = v_{atom} \cdot n_{atom} \cdot a^2 = \begin{matrix} 1.6\times10^{12}[s^{-1}] \\ 6.3\times10^{10} \end{matrix}$$

ρ=1.5g/cc, T=0.8eV
$t_{formation}$~600fs

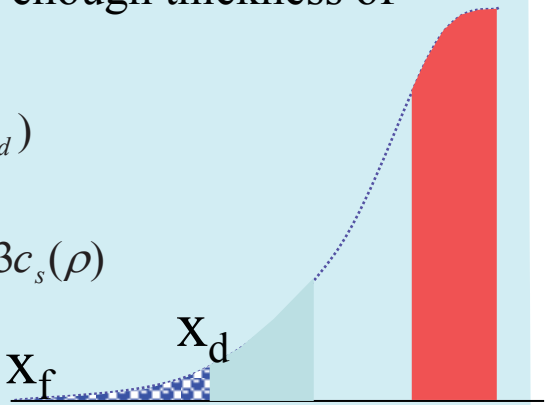
ρ=0.1g/cc, T=0.5eV
$t_{formation}$~16ps

Expansion time for enough thickness of droplet layer

$$\frac{x_d - x_f}{t_d} = R(\rho_d) + c_s(\rho_d)$$

$$R(\rho) = \int_0^{\rho} d\rho' \frac{c_s(\rho')}{\rho'} \cong 3c_s(\rho)$$

$$t_d \approx \frac{x_d - x_f}{4c_s(\rho_d)}$$



Why WDM physics?

Critical point data of Fluid metal

	atom	Tc[K]	P_c [MPa]	Vc [m^3/Mmol]	$Z_c=P_cV_c/RT_c$	ρ_c[g/cc]
static pressure	Hg	1750	167.3	34.8	0.40	5.80
	Cs	1651	9.25	351	0.203	0.38
	Rb	1744	12.45	293	0.218	0.29
	K	1905	14.8	--	--	0.18
	Se	1903	38.0	42.7	0.103	0.103
dynamic pressure	Na	2485 or 2210	25.6 ~ 24.8	76.7	0.095	0.30
	Sn	8720 or 9280	210 or 370	---	--	1.5?
	Pb	5400 or 5100	85 or 250	---	--	3.2
	In	6700?	400	---	--	2.1
	Mo	14000?	57	---	--	2.9
	W	23000? or 15000	>1000	---	--	--
	Many others	??	??	??	??	??

Information from Liquid metal physics

■many-body potential

$$V(\mathbf{r}_1,\cdots,\mathbf{r}_N)=\frac{1}{2}\sum_{i,j=1}^{N}{}'V_{\text{dimer}}\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)+V_{\text{mb}}(\mathbf{r}_1,\cdots,\mathbf{r}_N)$$

total potential energy in N-atom system

many-body potential

- *s-p mixing*
- *resonance of valence-bond structures (Pauling)*

calculate $V_{\text{mb}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ for *selected geometries* of Hg_N clusters

--- *spin-orbit diatomics-in-molecules method* [H.K., Chem. Phys. Lett. **425**, 205 (2006)]

D_{3h}	T_d	D_{3h}	D_{5h}	O_h
N=3	N=4	N=5	N=7	N=13
z=2	z=3	z=3.6	z=4.29	z=5.54

breathing motion

average coordination number

nearest-neighbor distance

$$\frac{V_{\text{mb}}(z,r_{\text{nn}})}{N}$$

H. Kitamura

many-body interaction: crystalline solids (metallic)

potential energy per atom

electron gas energy, etc.

$$\frac{V}{N}=\frac{1}{2}\left[12\Phi_{\mathrm{eff}}\left(r_{\mathrm{nn}}\right)+6\Phi_{\mathrm{eff}}\left(\sqrt{2}r_{\mathrm{nn}}\right)\right]+\frac{U_0(n)}{N}$$

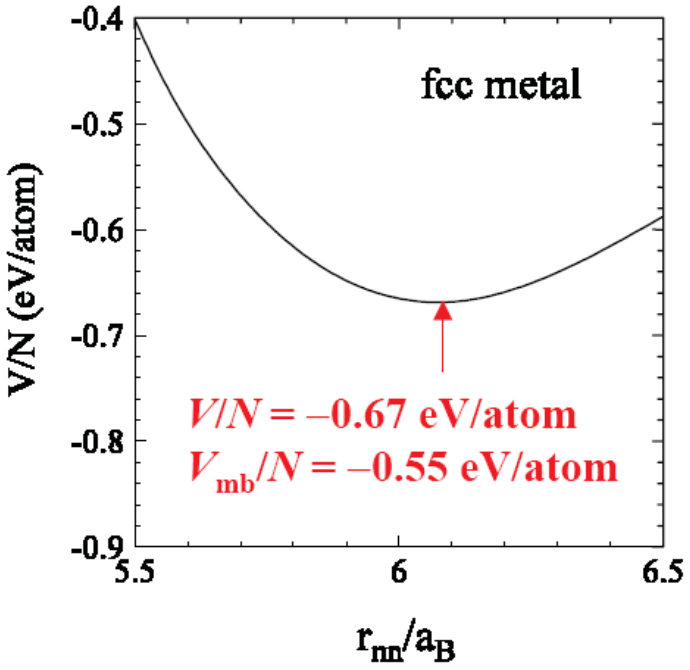
1st neighbor **2nd neighbor**

core radius

$$\Phi_{\mathrm{eff}}\left(r\right)=\frac{(Ze)^2}{r}+\frac{1}{2\pi^2}\int_0^\infty dk k^2\,\frac{4\pi(Ze)^2}{k^2}\left[\frac{1}{\varepsilon_{\mathrm{e}}(k)}-1\right]\cos^2(kR_{\mathrm{c}})\frac{\sin(kr)}{kr}$$

$$+A\frac{e^2}{a_{\mathrm{B}}}\exp\left(-B\frac{r}{a_{\mathrm{B}}}\right)$$

electron screening



effective potential between Hg^{2+} ions (Z=2)

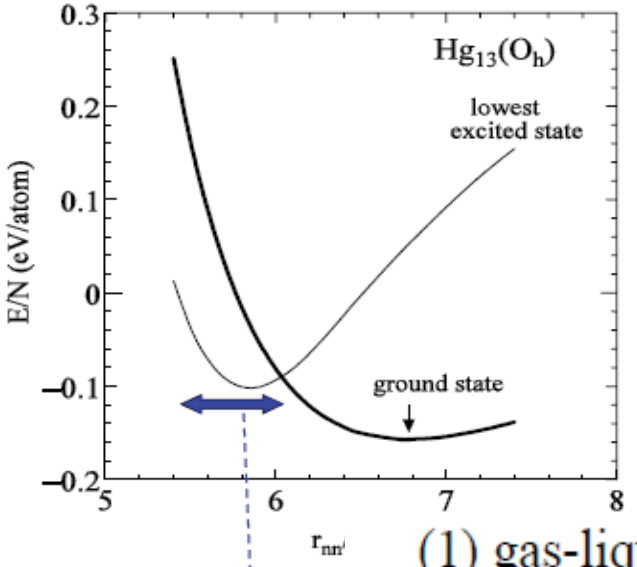
Chekmarev et al., Phys. Rev. E **59**, 479 (1999)

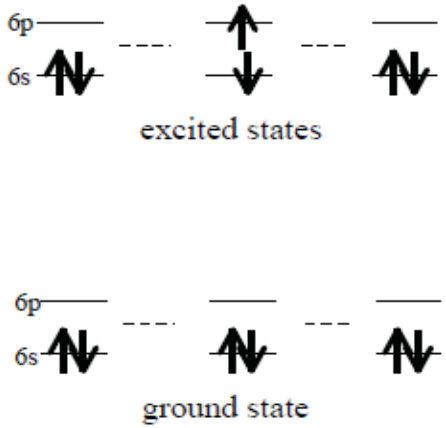
H. Kitamura, 2008 WDM school

potential energy curve of Hg_{13} (cuboctahedron)

Theoretical investigation of 2ϕ region

from H. Kitamura

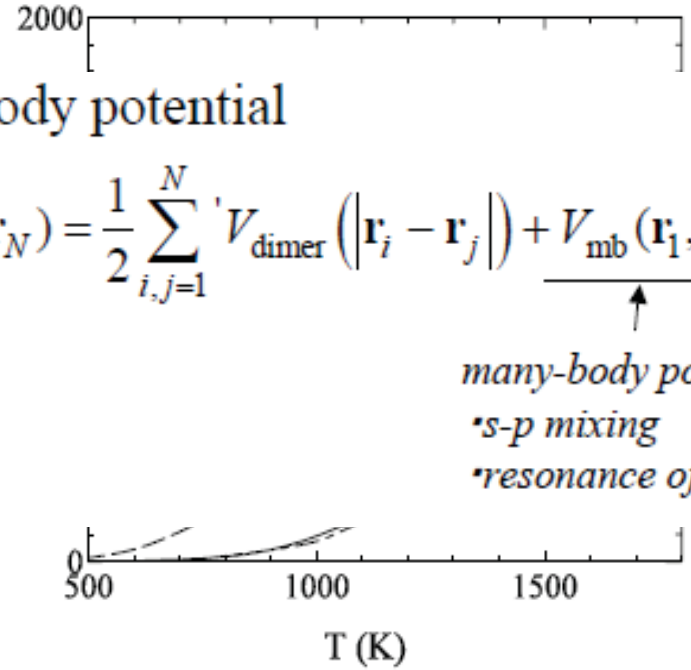


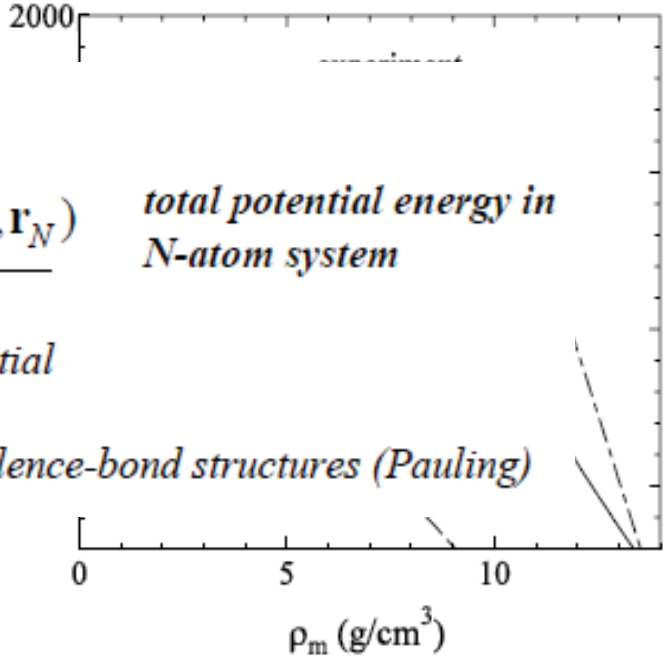


(1) gas-liquid coexistence curves

"excitonic g

--- large adv





■ many-body potential

$$V(\mathbf{r}_1,\cdots,\mathbf{r}_N)=\frac{1}{2}\sum_{i,j=1}^{N}{}' V_{\text{dimer}}\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)+V_{\text{mb}}(\mathbf{r}_1,\cdots,\mathbf{r}_N)$$

total potential energy in N-atom system

many-body potential

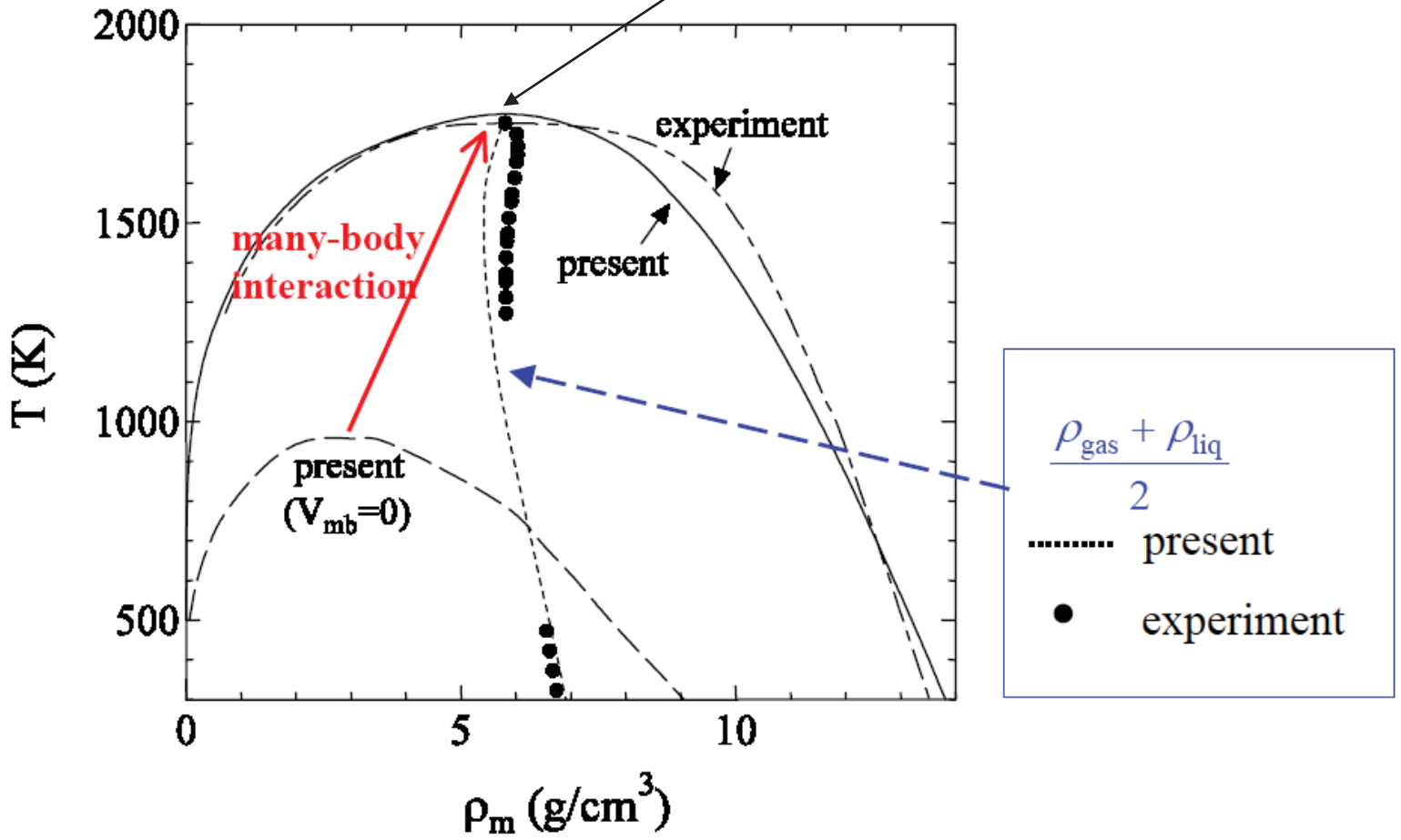
- *s-p mixing*
- *resonance of valence-bond structures (Pauling)*

Modeling for Liquid metal

- gas-liquid coexistence curves

$P(\rho_{gas}, T) = P(\rho_{liquid}, T)$ pressure

$G(\rho_{gas}, T) = G(\rho_{liquid}, T)$ Gibbs free energy

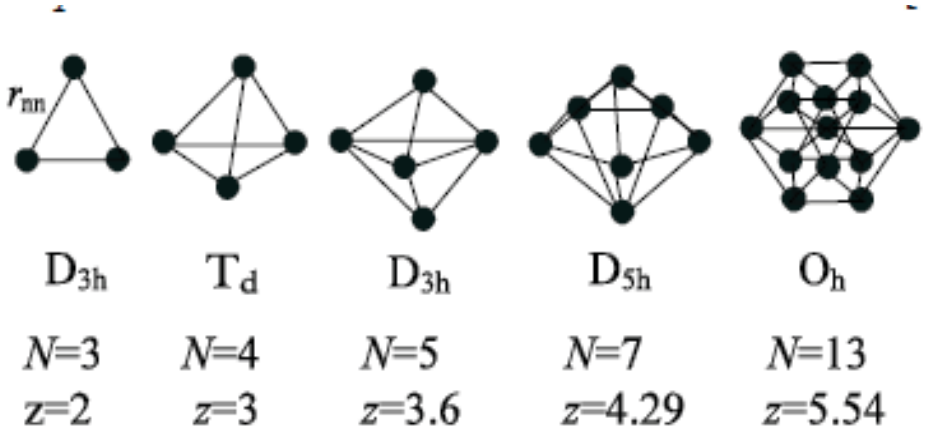


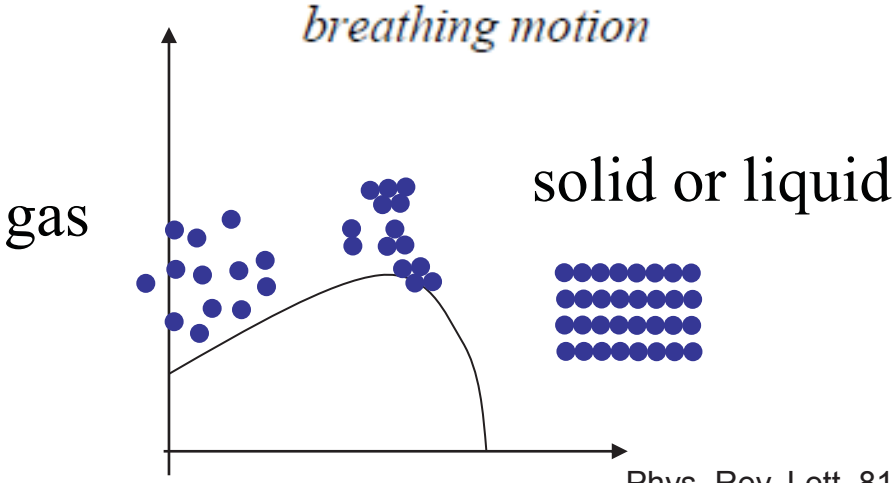
H. K., J. Phys.: Condens. Matter **19**, 072102 (2007)

H. Kitamura, 2008 WDM school

Conductivity problem

Photoelectron spectrum of Hg
(band gap information)
(single electron detection)





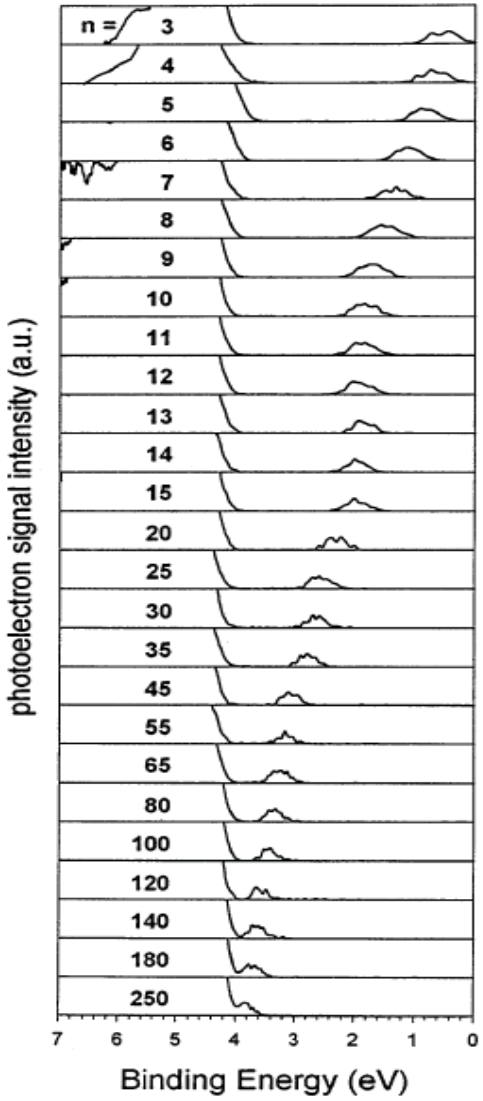
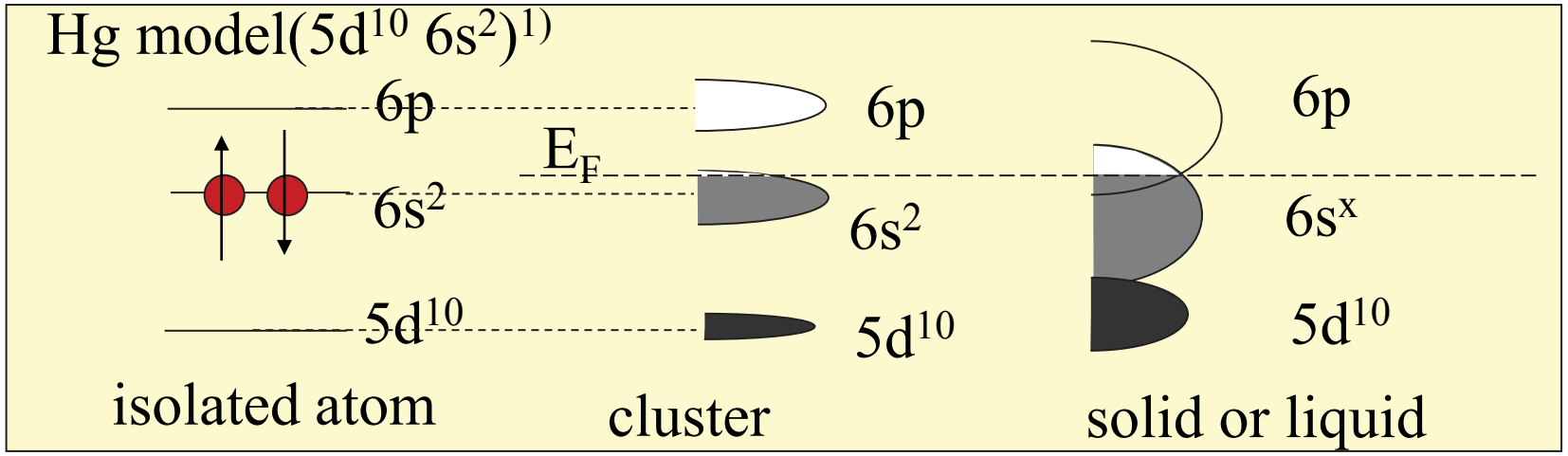


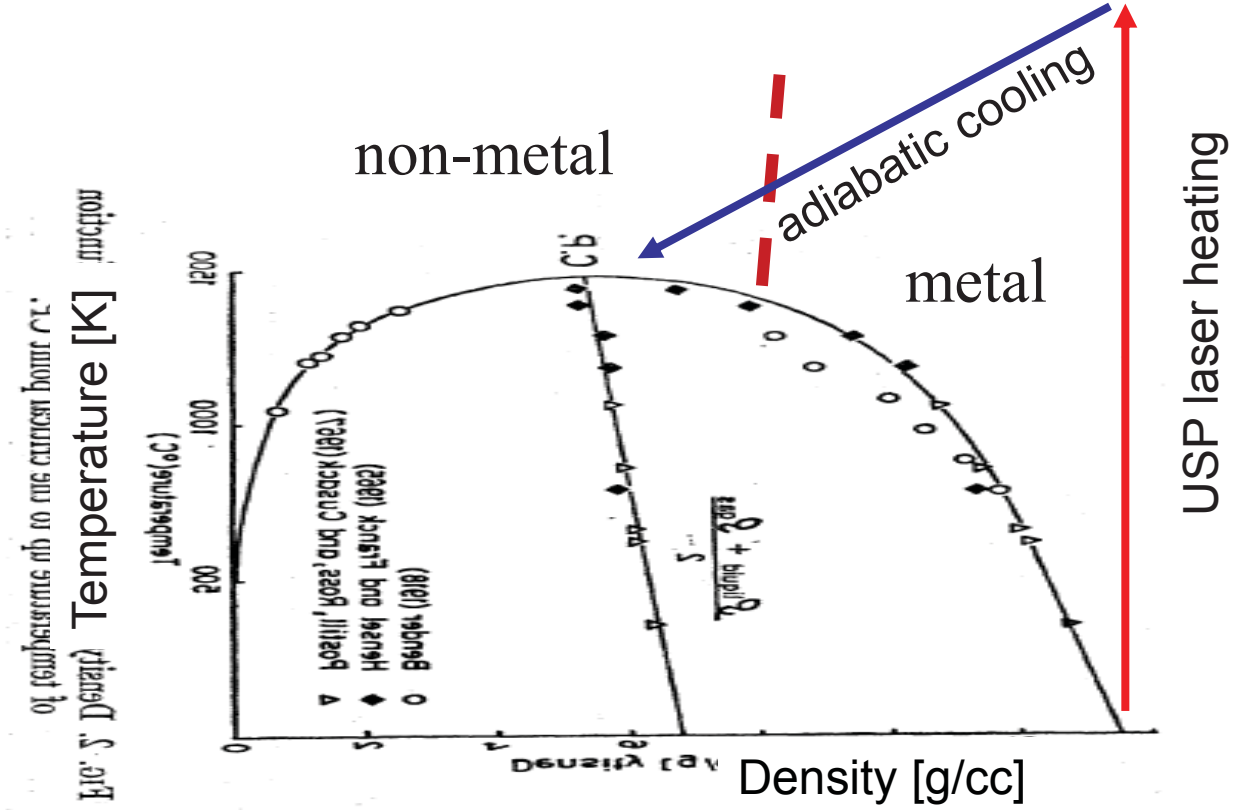
FIG. 2. Photoelectron spectra of Hg^-_n in the size range of $n = 3$–250 taken with 7.9 eV laser excitation. The spectra are scaled and truncated to show a constant intensity of the single peak of the detached $6p$ electron. The fine structure of the $6p$ peaks is due to statistical scatter of photoelectron counts.

Phys. Rev. Lett. 81, 3836–3839 (1998)

Metal-Nonmetal transition in Hg



1)H. Haberland, et al., PRL, vol.69, p.3212

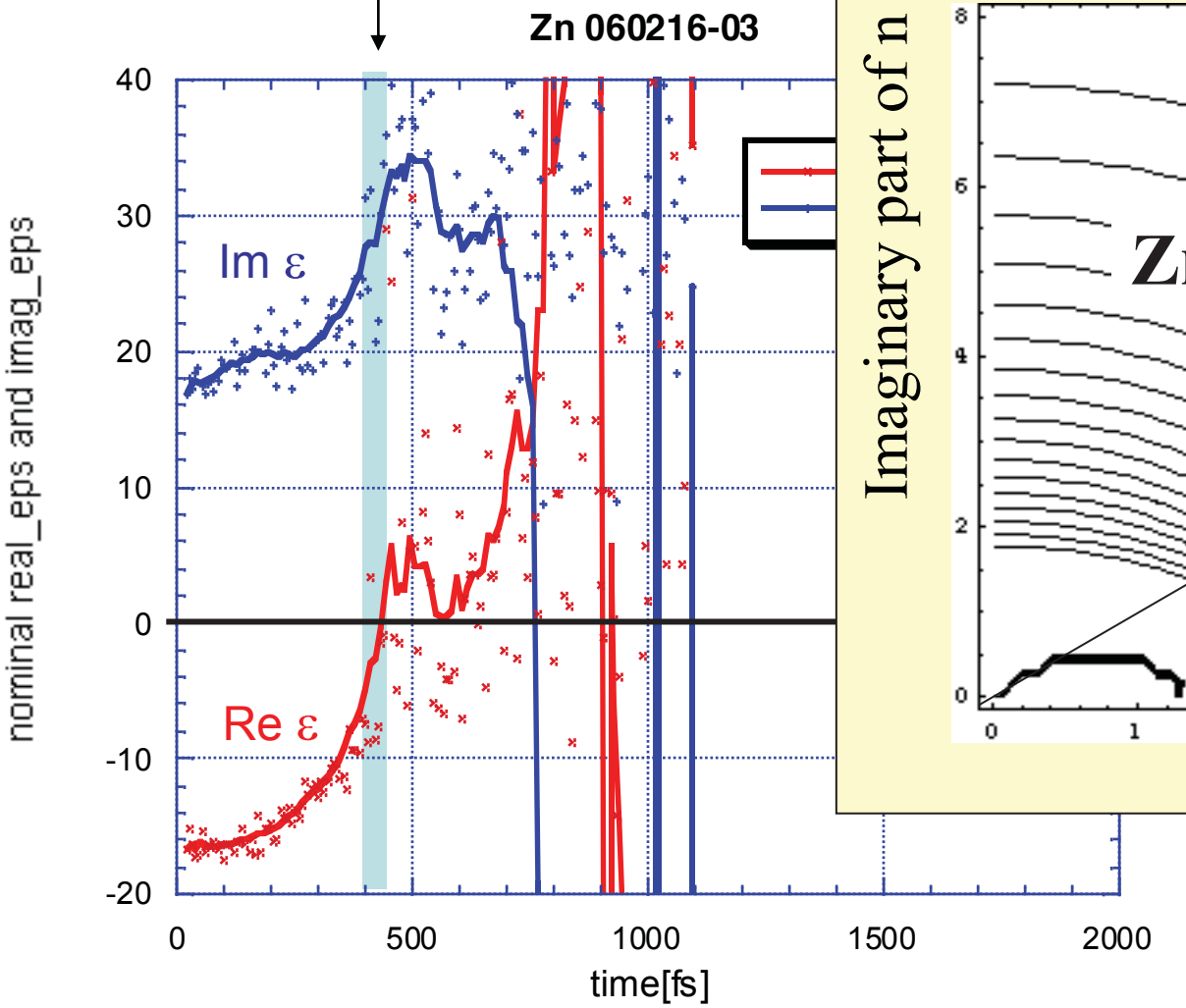


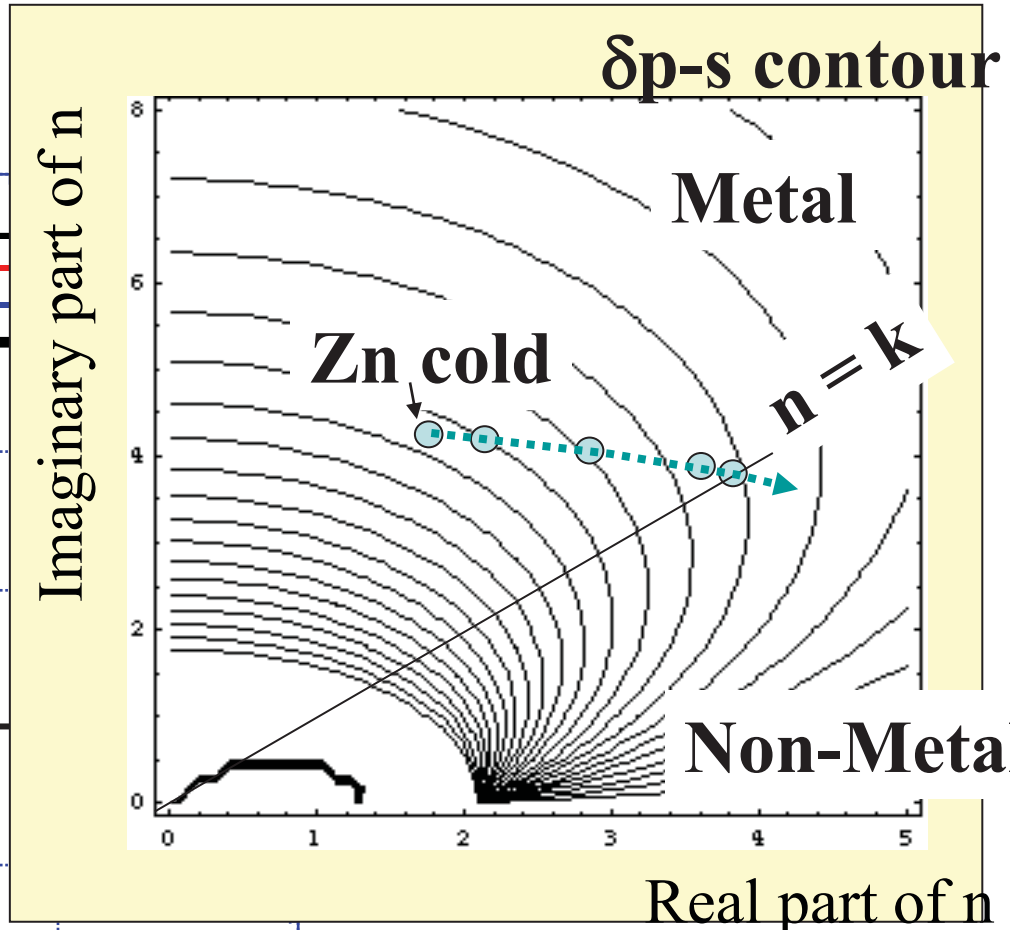
High temperature Zn goes to non-metal condition.

Hg: $5d^{10}\ 6s^2$

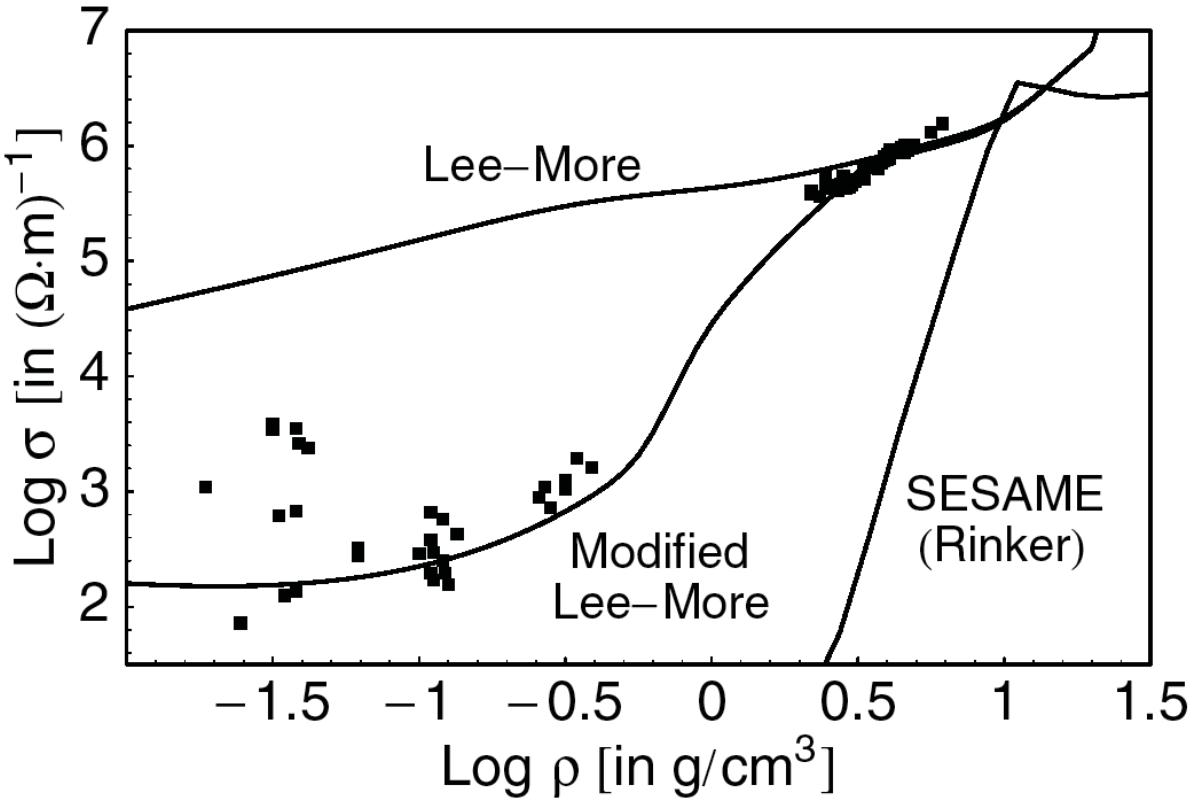
Zn: $3d^{10}\ 4s^2$

Onset time of expansion

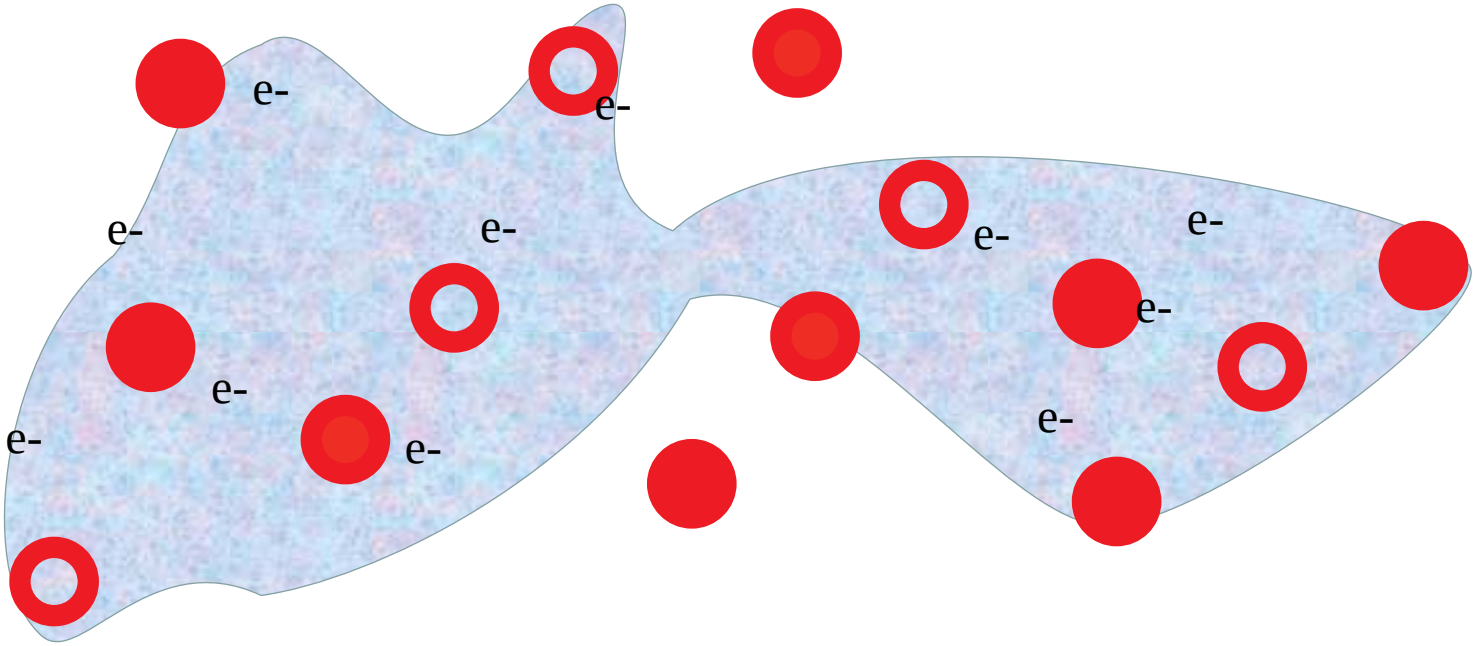


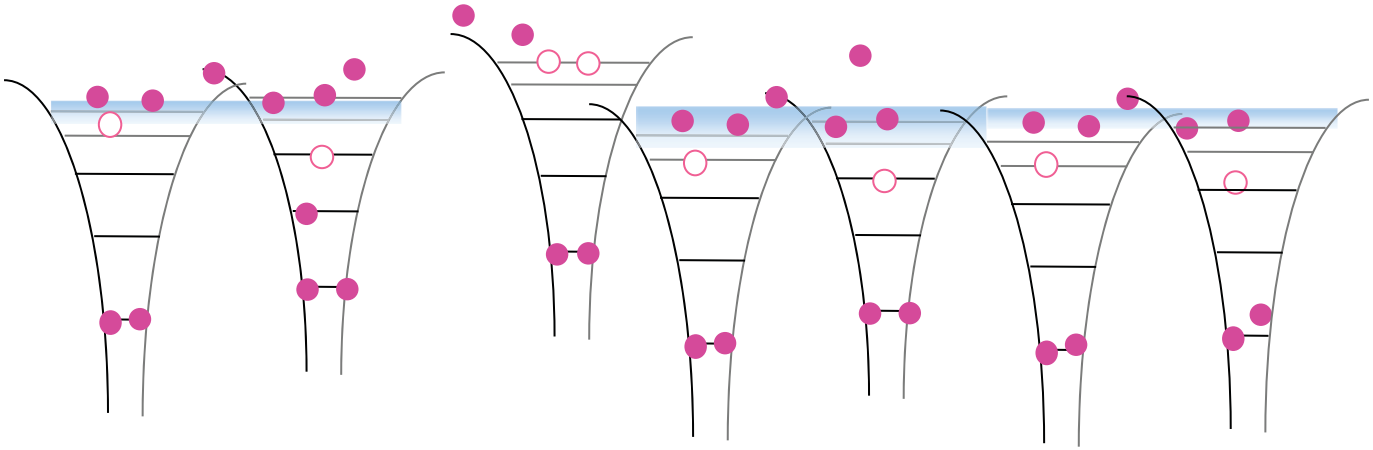


The M-NM transition in Hg type is different from large reduction of DC conductivity in Cu, Au, Al



Electronic system is different between Hg and Cu.


e-
e-
e-
e-
e-
e-
e-
e-
e-
e-

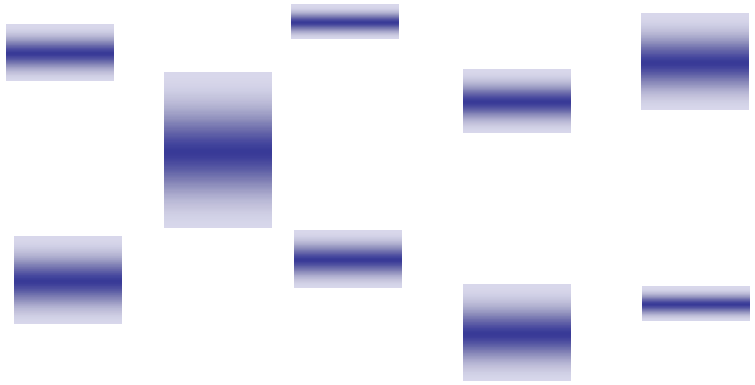


Possible explanation

Private communications with RMM

Switching of σ

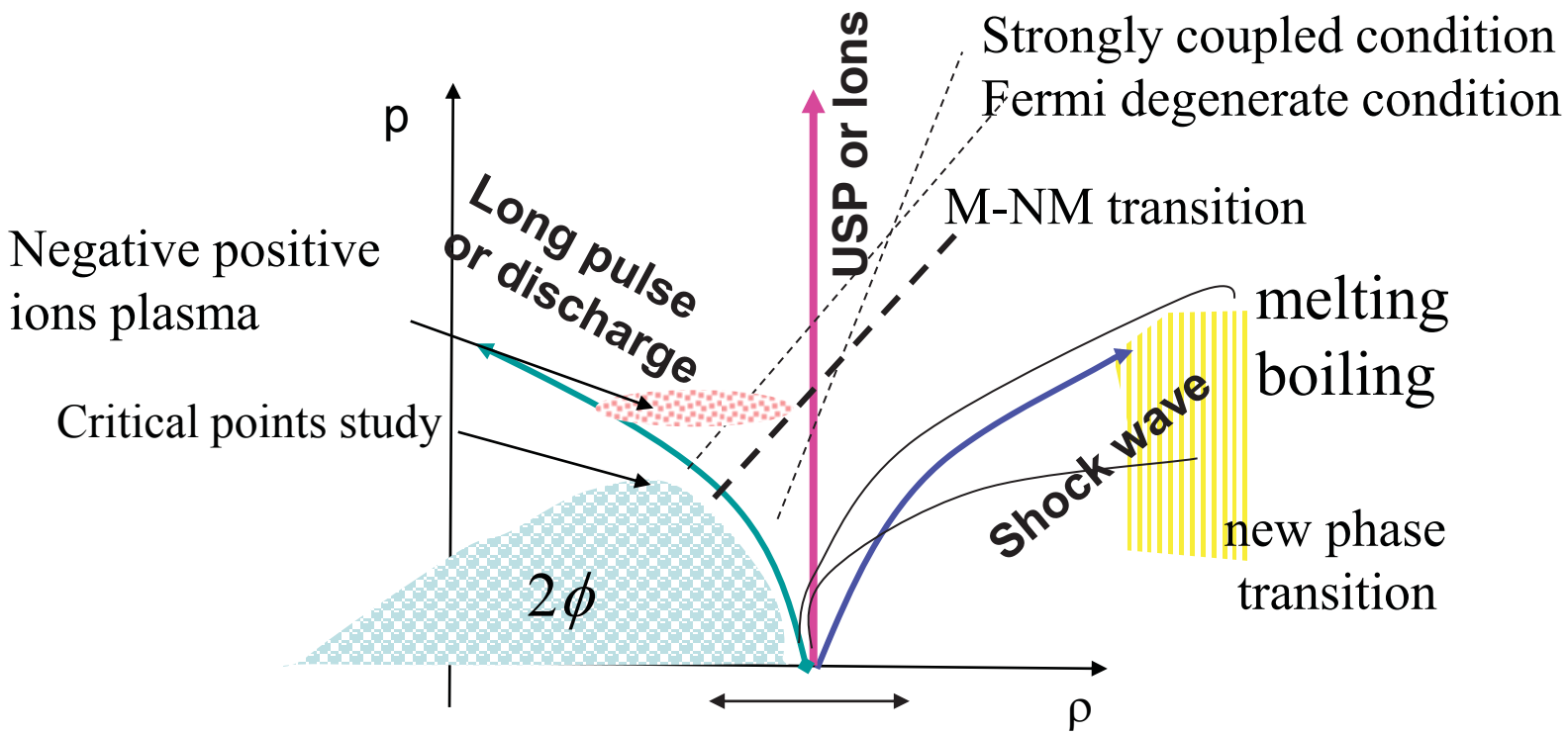
low-σ state
Inhomogenity and disorder
inhibit charge transfer



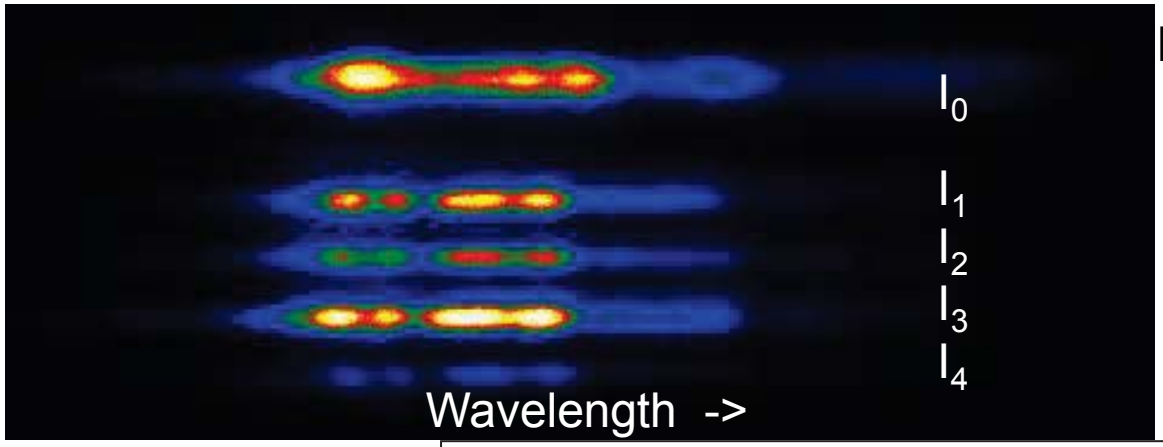
high-σ state
Collisional widths
enable charge transfer

Dynamic line width control conduction
<=> hopping conduction of amorphous semiconductors

A lot of varieties method of WDM creation

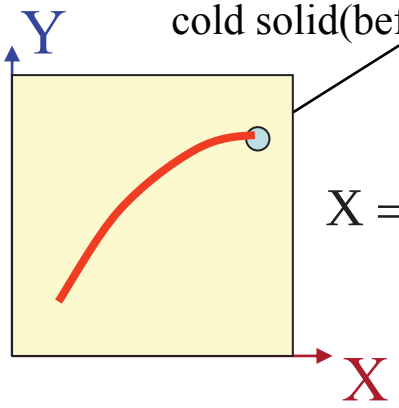


Start points:
Solid, liquid, gas, low density foam?

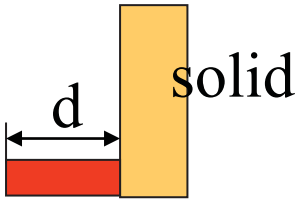

I_0
I_1
I_2
I_3
I_4
Wavelength ->
Droplet lens
Photonic crystal fiber
+
ω
Ti:Sapphire ultra-short-pulse laser
pump beam
KrF amplifier
3ω
Photonic crystal fiber
White light probe
4-detectors ellipsometric measurement system
Pol1
Pol2
target
I_1
I_2
I_3
I_4
Imaging Spectrometer + Gated ICCD camera
WDMを調べるには？

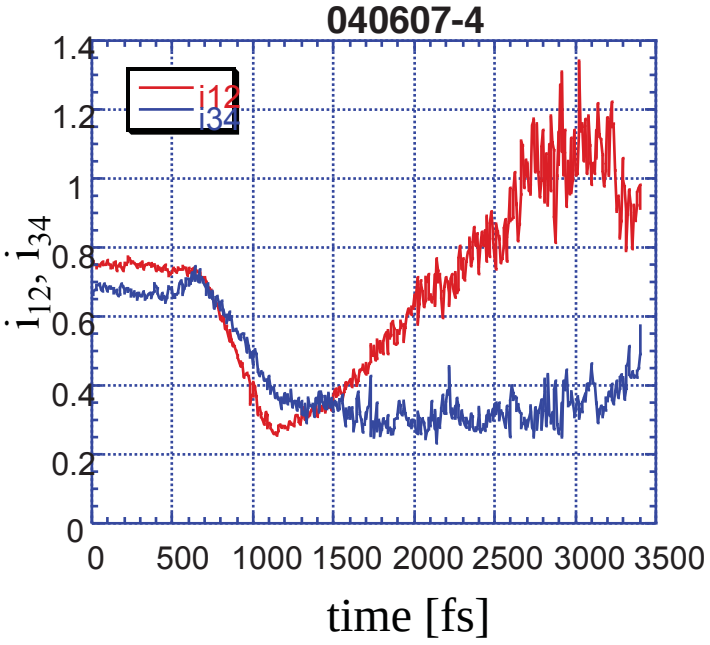
Change of polarization state of probe beam with target heating

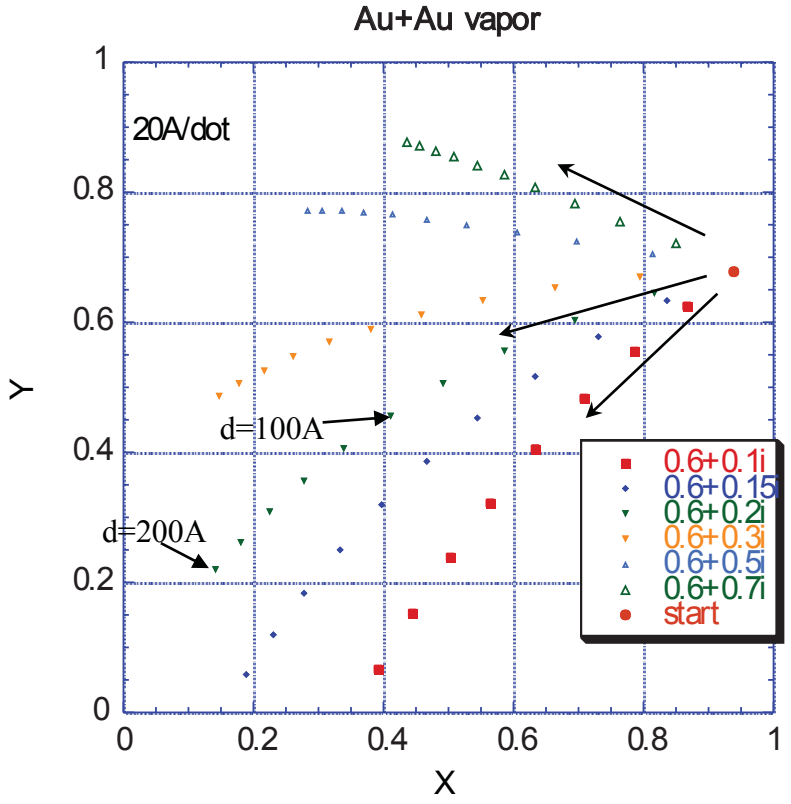
$$Y = \frac{I_3 - I_4}{I_3 + I_4} = \frac{2|R_S||R_P|\sin(\delta)}{|R_S|^2 + |R_P|^2}$$



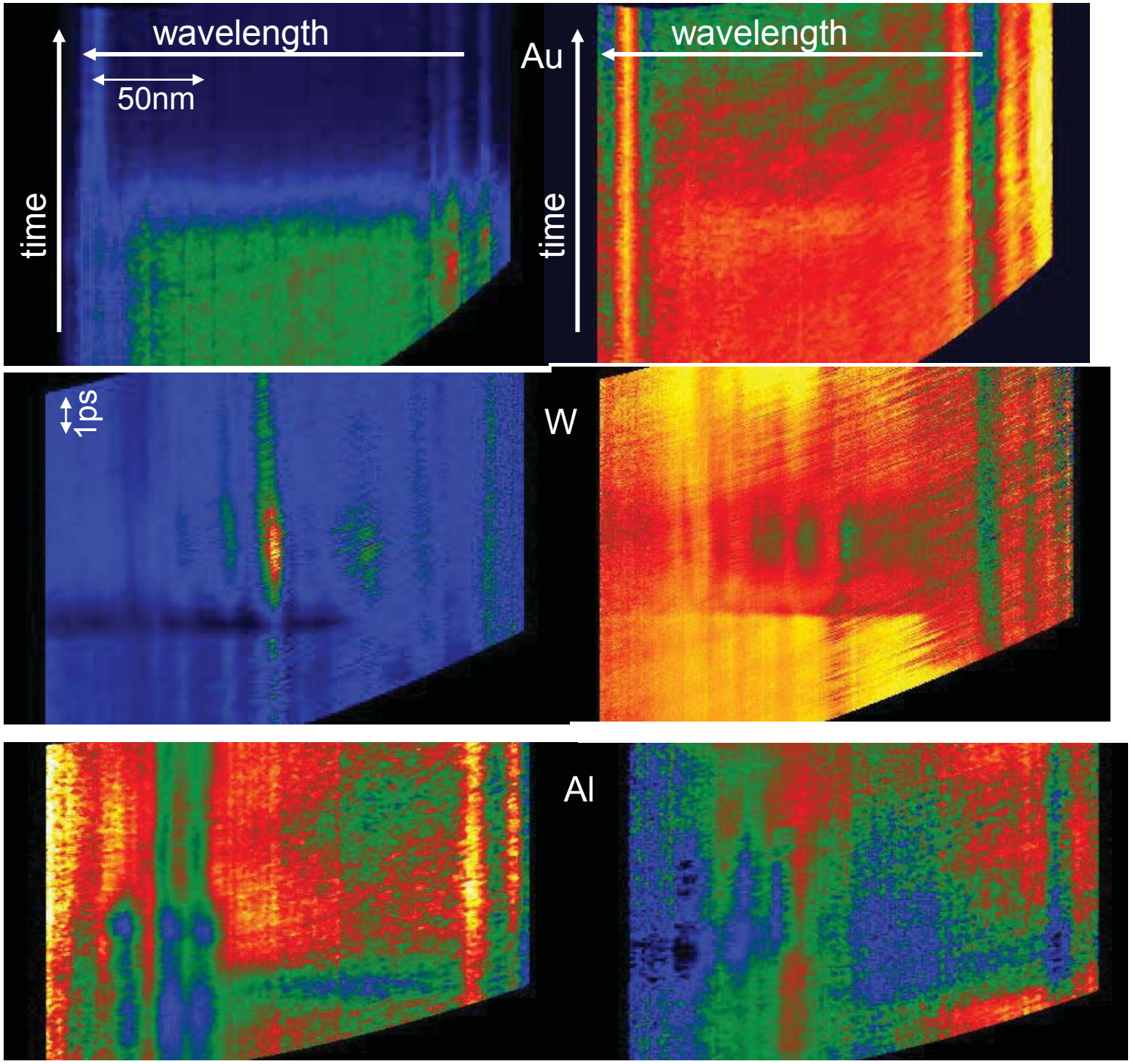
$$X = \frac{I_2}{I_1} = \frac{|R_p|^2}{|R_s|^2}$$







Very sensitive to optical constant and thickness of plasma

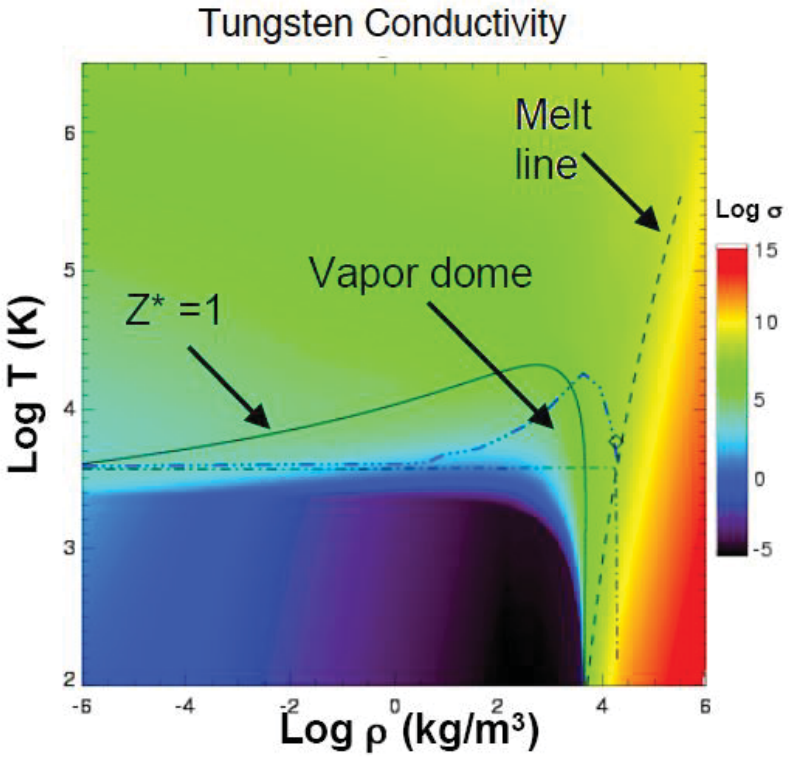

wavelength
50nm
time
Au
wavelength
time
1ps
W
Al

More Detailed modeling

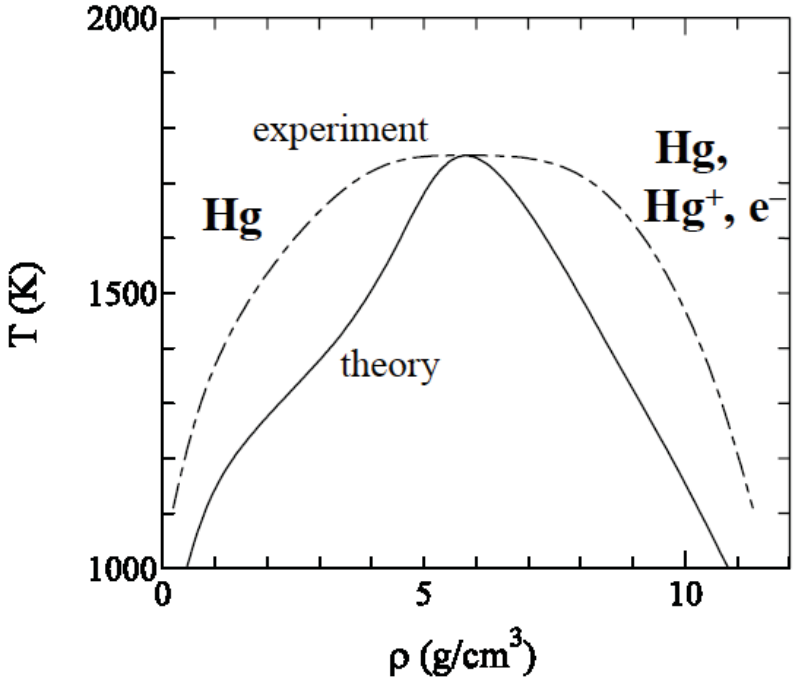
Question: Can we change two-phase boundary with ionization and rich excitation?

(including non-equilibrium effect)

W: Tc~1.1~1.5eV, IP=7.98eV



M.D, 2008 wdm school



The coexistence curve is ***too sharp.***

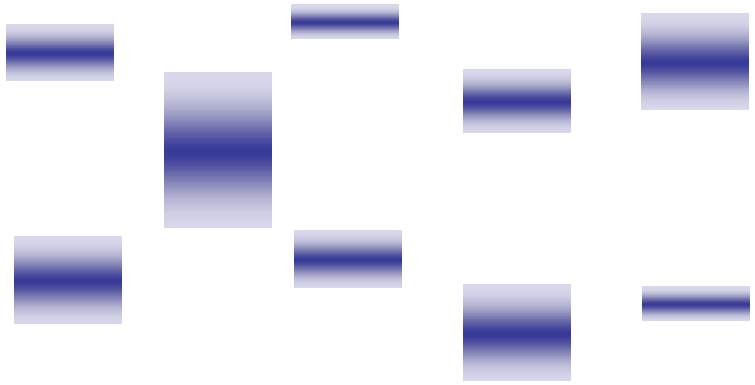
H.K., J. Phys.:Condens. Matter **15**, 6427 (2003)

New approach of modeling

Private communications with RMM

Switching of σ

low-σ state
Inhomogenity and disorder
inhibit charge transfer



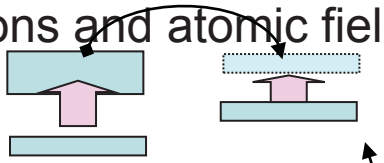
high-σ state
Collisional widths
enable charge transfer

Dynamic line width control conduction
<=> hopping conduction of amorphous semiconductors

Private communications with RMM

Microfield analysis

level-broadening and shifting occurs due to the motion of electrons and atomic field



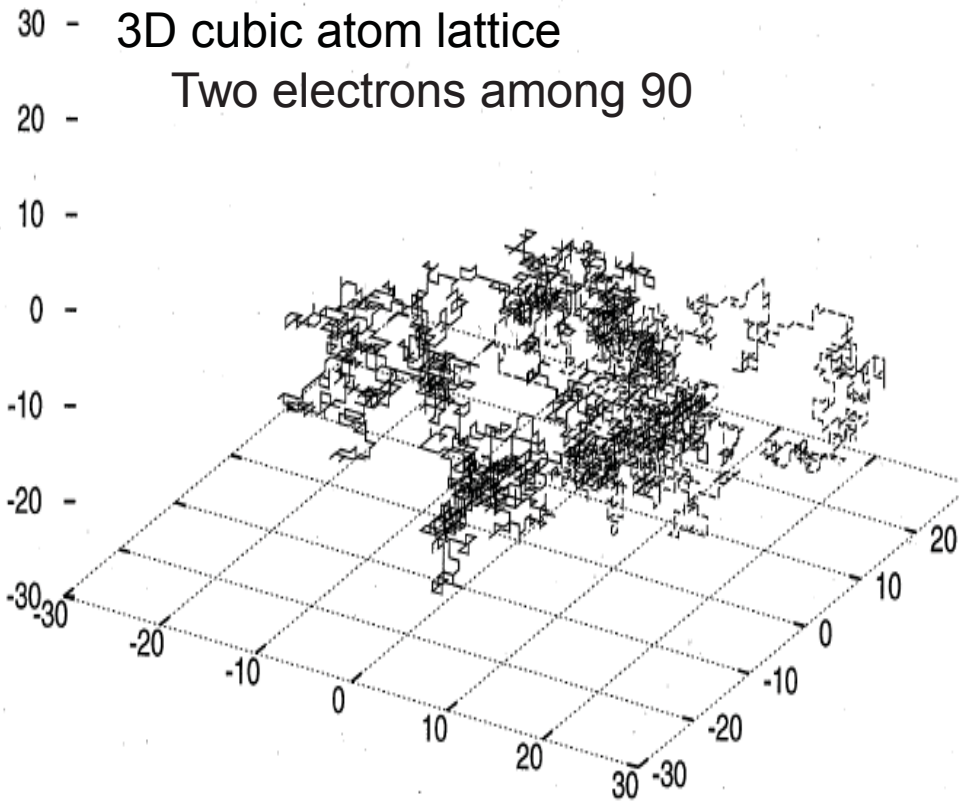
If ΔE(width of states) > δE (energy space),
the transition between metal and insulator may be occurred.

FT

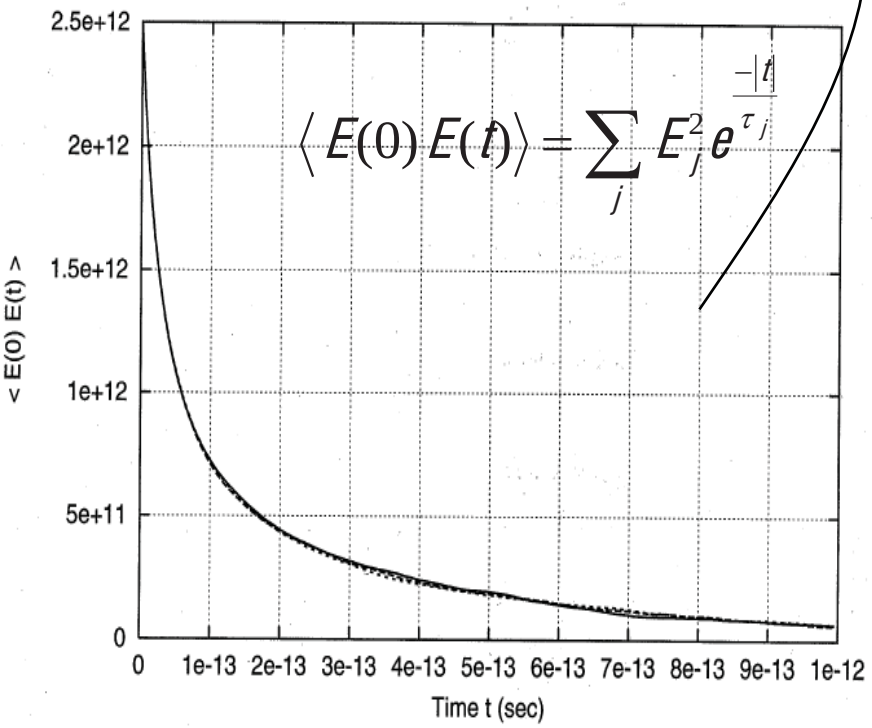
High density, high temperature ⟺ Low density, low temperature

3D cubic atom lattice

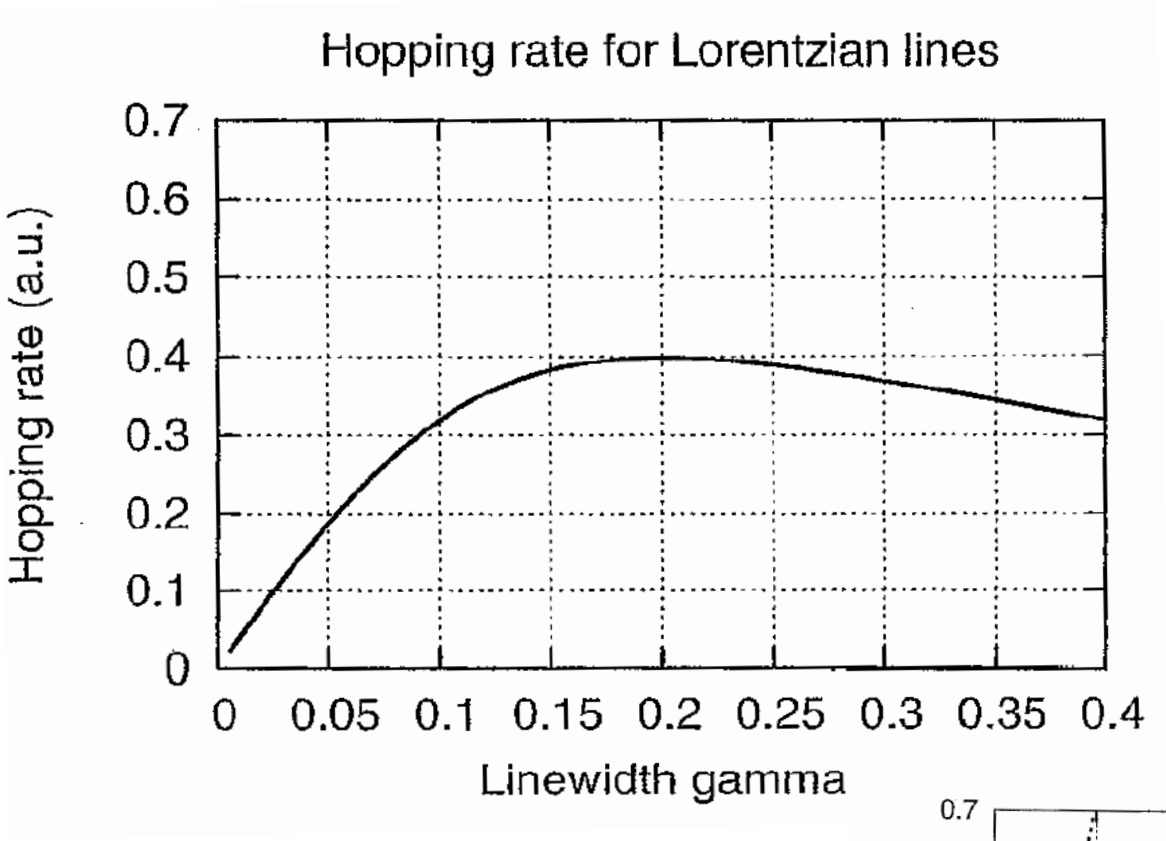
Two electrons among 90

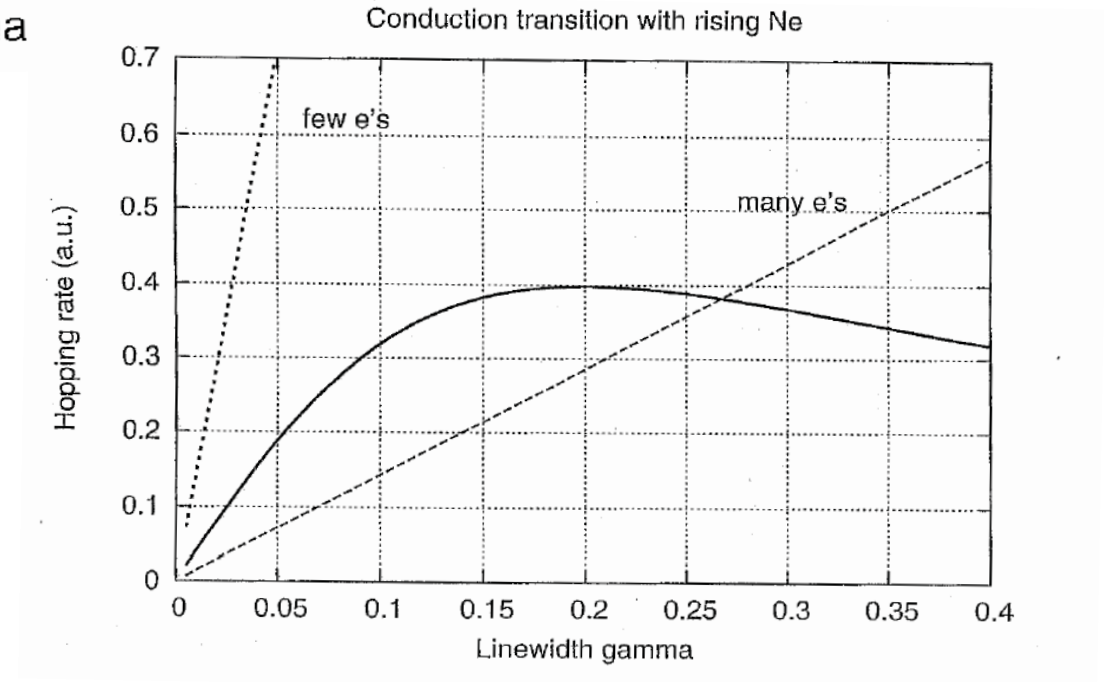


E-field autocorrelation



Private communications with RMM





Simple model for EOS

Empirical formula with Van der Waals' law

pressure $$p = \frac{\rho k T}{A M_p (1 - b\rho)} - a\rho^2$$

specific energy $$\varepsilon = \frac{3}{2}\frac{kT}{AM_p} - a\rho$$

specific entropy $$S = \frac{k}{AM_p}\log\left(AM_p \frac{1 - b\rho}{\rho \lambda^3} \right)$$

Thermal deBrogie wevelength $$\lambda = \sqrt{\frac{h^2}{2\pi A M_p k T}}$$

Helmholtz free energy $$F = \varepsilon - TS$$

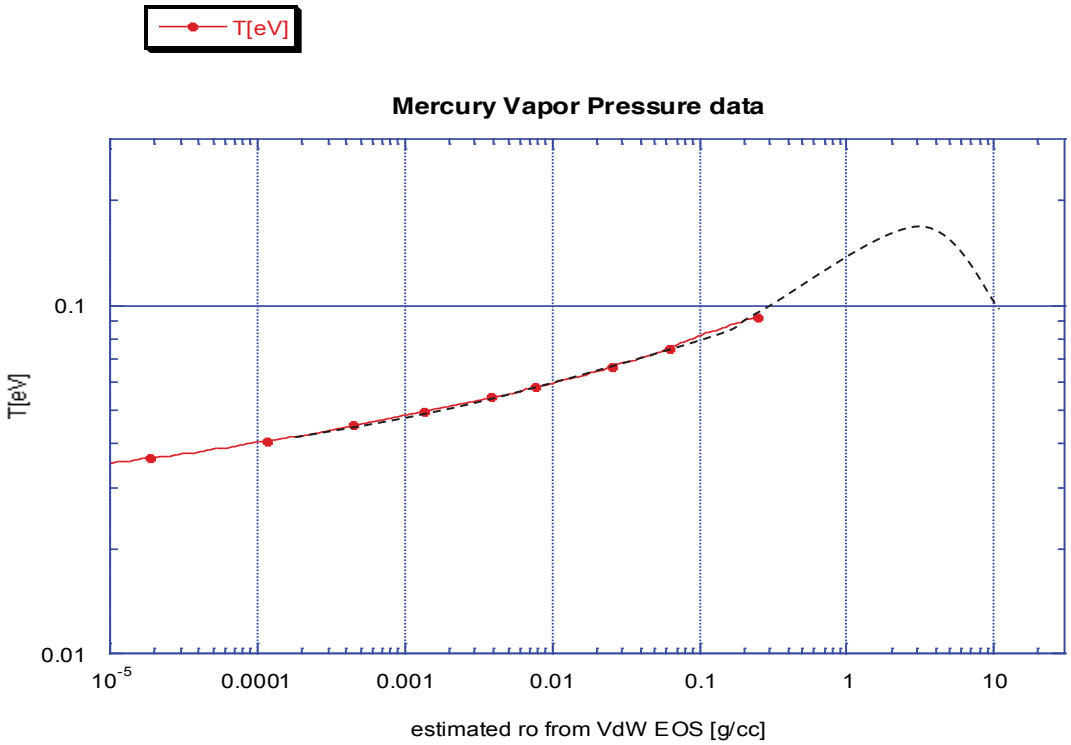
Critical density and temperature $$\rho_c = \frac{1}{3b} \qquad kT_c = \frac{8a}{27b} AM_p$$

Critical pressure and specific energy $$p_c = \frac{a}{27b^2} \qquad \varepsilon_c = \frac{a}{9b}$$

For water

ρ_{crit}	=	0.396 g/cm^3		0.317 g/cm^3
T_{crit}	=	.05578 eV	(adjusted!)	.05578 eV
p_{crit}	=	44.37 J/cm^3		22.09 J/cm^3
E_{crit}	=	112 J/gram (wrt gas)		2.032 kJoule/gram (relative to liquid)
				- 346 J/gram (relative to the gas)
S_{crit}	=	4.335 J/g-C		4.435 J/g-C

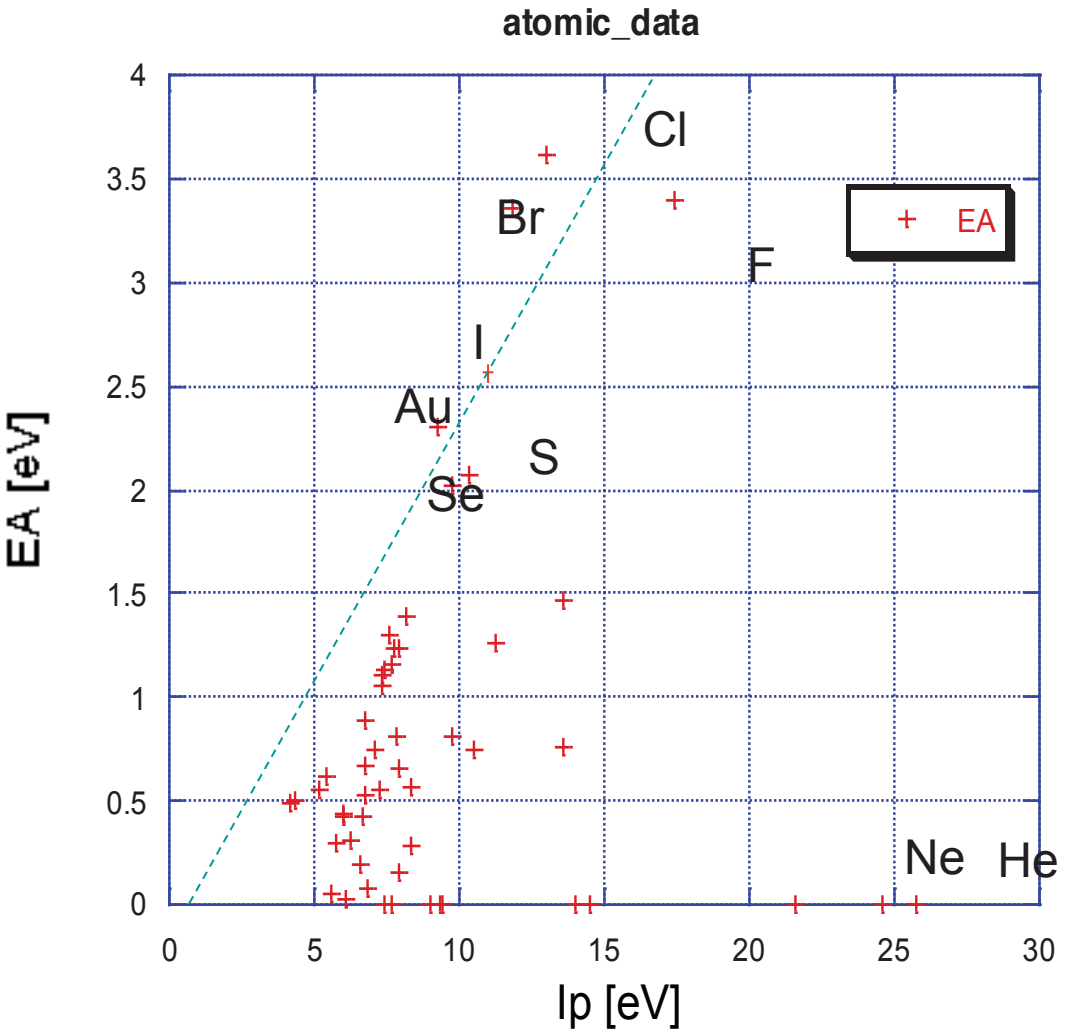
For Hg

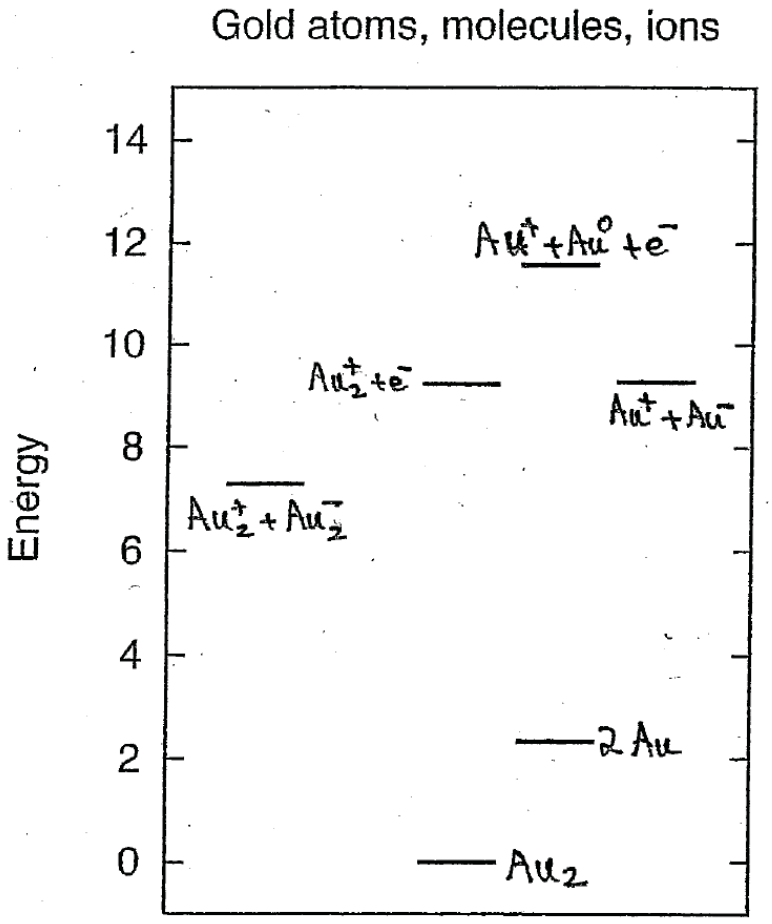


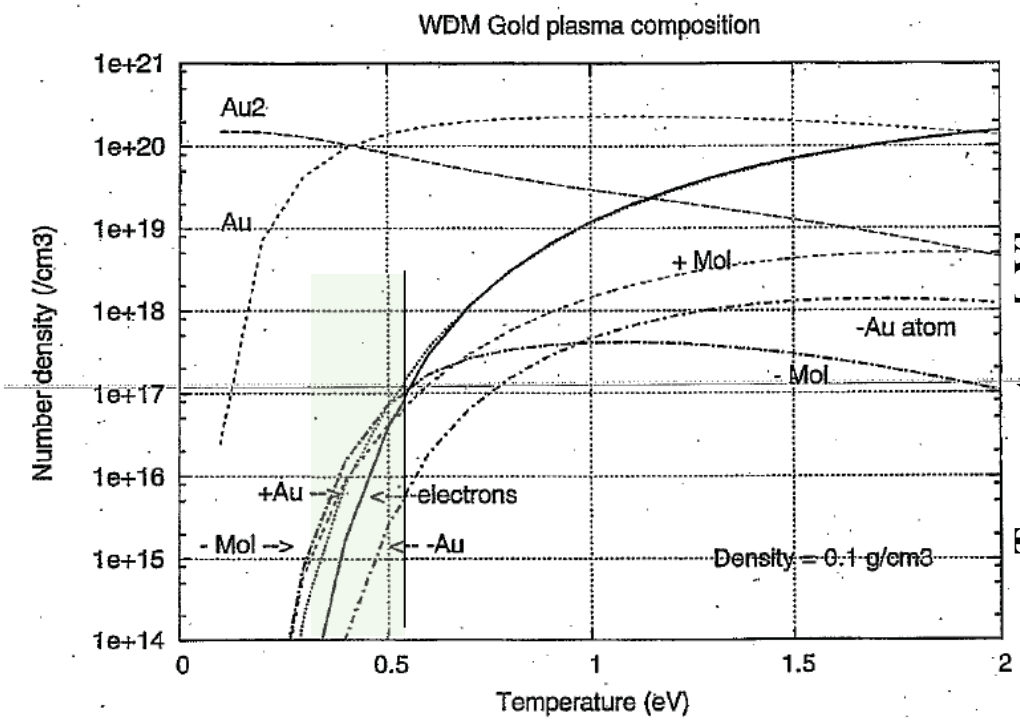
Other’s feature we should include

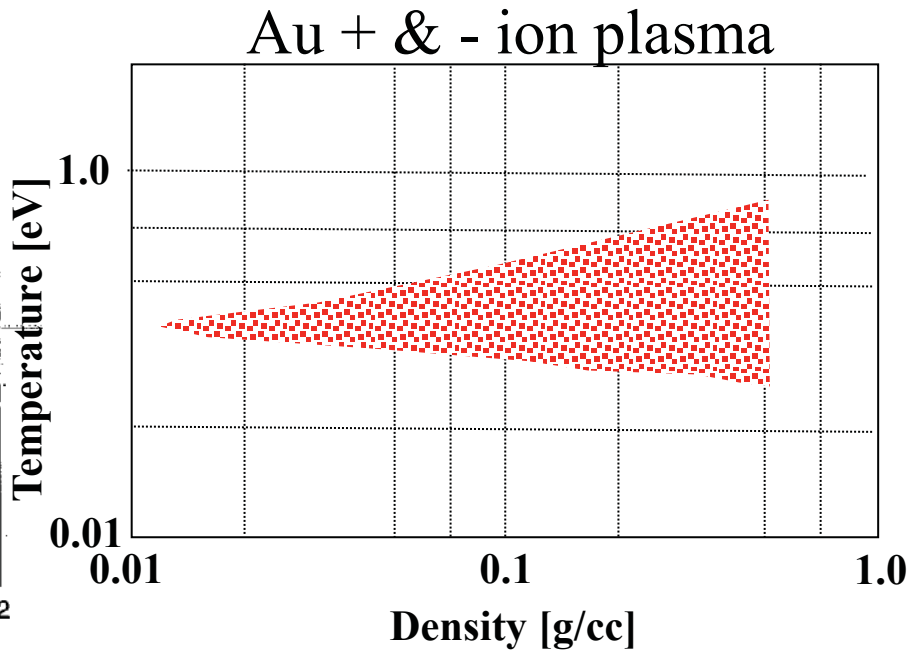
Electron affinity

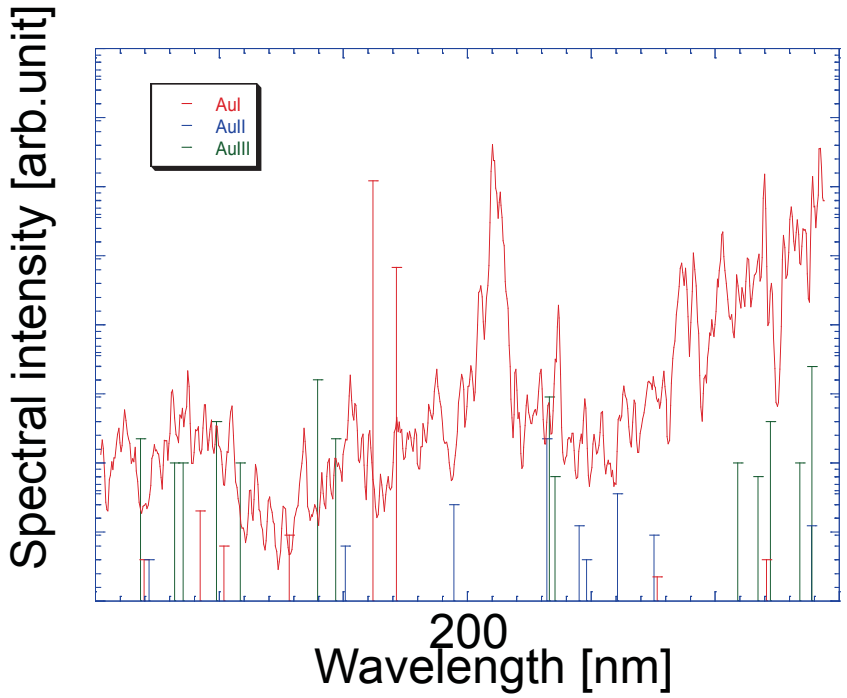
Including negative ion and its pairing

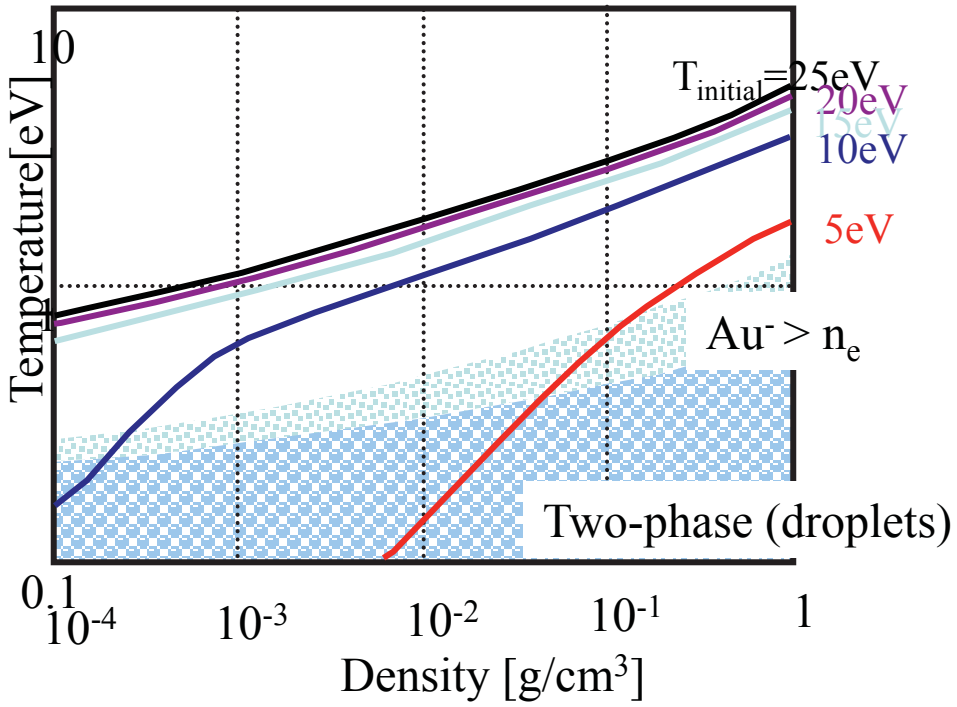





WDM Gold plasma composition
Number density (/cm3)
Temperature (eV)
Au2
Au
+ Mol
-Au atom
- Mol
+Au
-electrons
- Mol -->
-Au
Density = 0.1 g/cm3


Au + & - ion plasma
Temperature [eV]
Density [g/cc]


Spectral intensity [arb.unit]
AuI
AuII
AuIII
200
Wavelength [nm]


Temperature[eV]
T initial=25eV
20eV
15eV
10eV
5eV
Au- > ne
Two-phase (droplets)
Density [g/cm3]

Continuum lowering should be changed with negative ions.

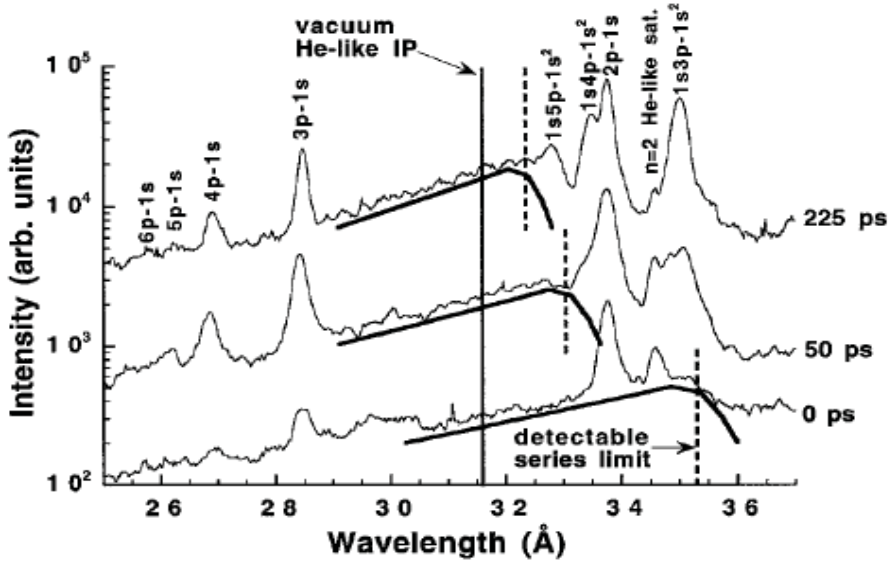
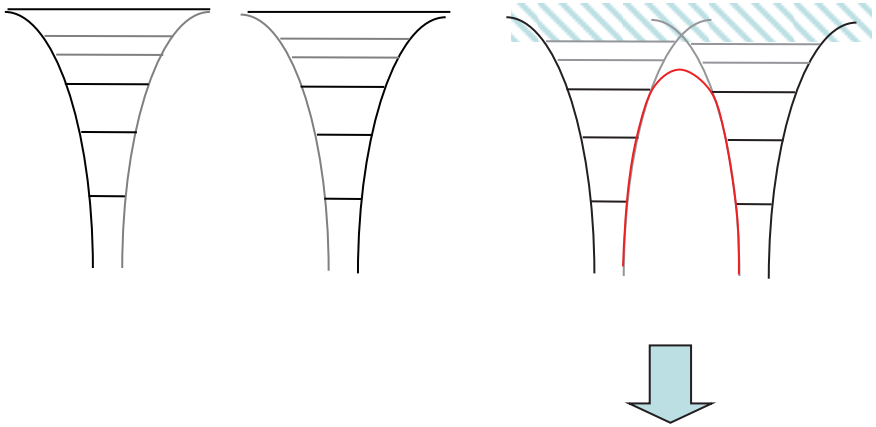


FIG. 1. Lineouts from the time-resolved spectra taken at $t = 0$, 50, and 225 ps. The He-like $np1s$-$1s^2$ ($n > 3$) and H-like np-$1s$ line emissions are identified, as well as the $n = 2$ He-like satellites to the H-like $2p$-$1s$ line. The free-bound continuum and the detectable series limit are drawn on each lineout. Considerable He-like $2p1s$-$1s^2$ emission at 40.268 Å was seen in each spectrum, but is not included here for better emphasis on the spectral region between 25 and 37 Å. The three lineouts are offset vertically for better viewing.

M.Nantel, PRL, 80 (1998)

$$\Delta E = \sum_j N_j \left(-\frac{9}{10} \frac{Z_j^2 e^2}{R_j} \right)$$

$$\left(\frac{4\pi}{3} R_j^3 \right) n_e = Z_j$$



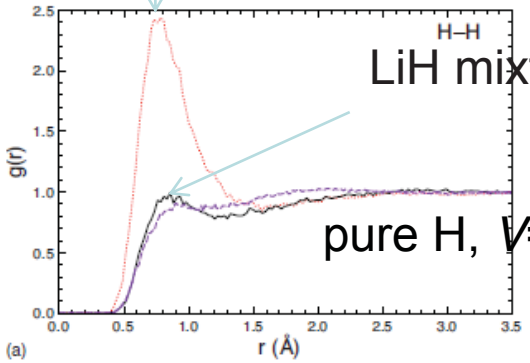
Creation of negative ions

Mixing problem

D. A. Horner, J. D. Kress, and L. A. Collins, PHYSICAL REVIEW B **77**, 064102 2008

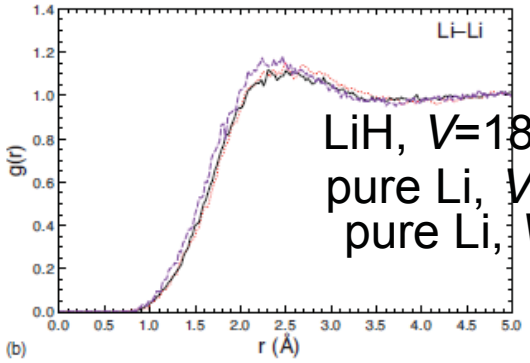
Examination of mixing rules

pure H V=1824 Å^3



LiH mixture V=1824 Å^3

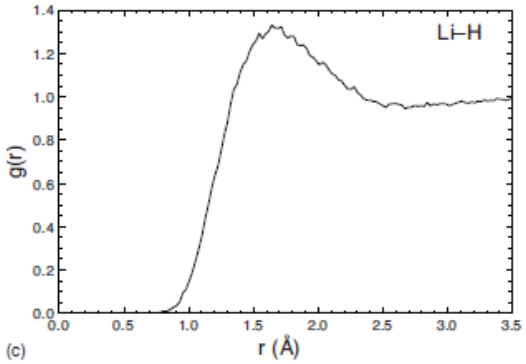
pure H, V=424 Å^3



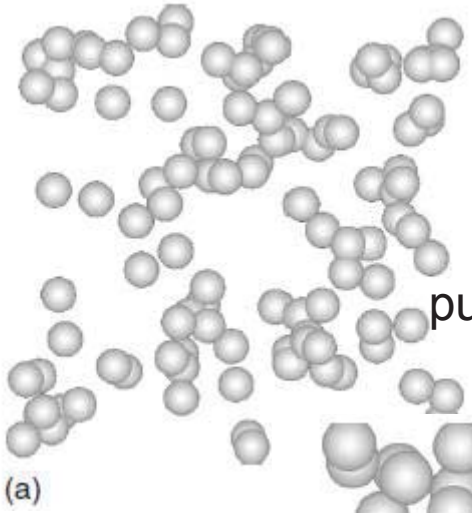
LiH, V=1824 Å^3

pure Li, V=1824 Å^3

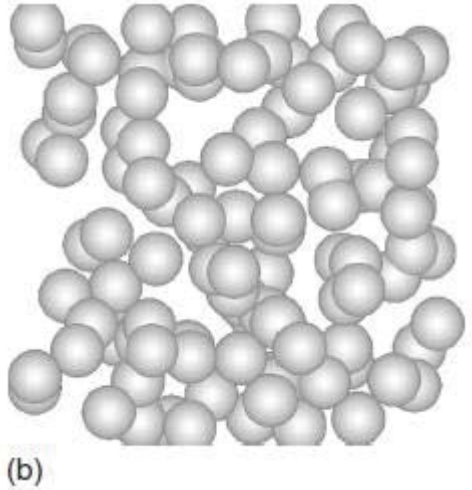
pure Li, V=1400 Å^3



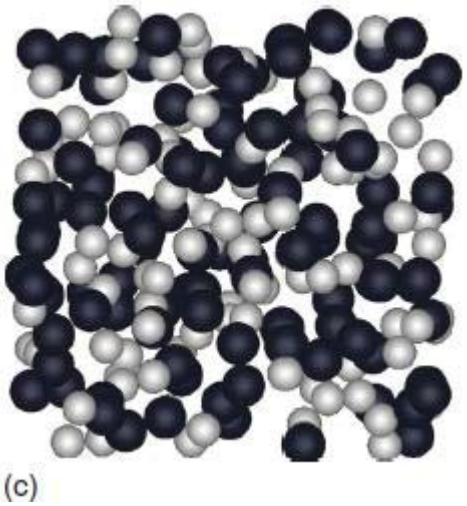
1.0 eV , 0.7874 g/cm3.



pure H V=1824 Å^3



pure H, V=424 Å^3



pure H, V=424 Å^3

Opacity in mixing condition

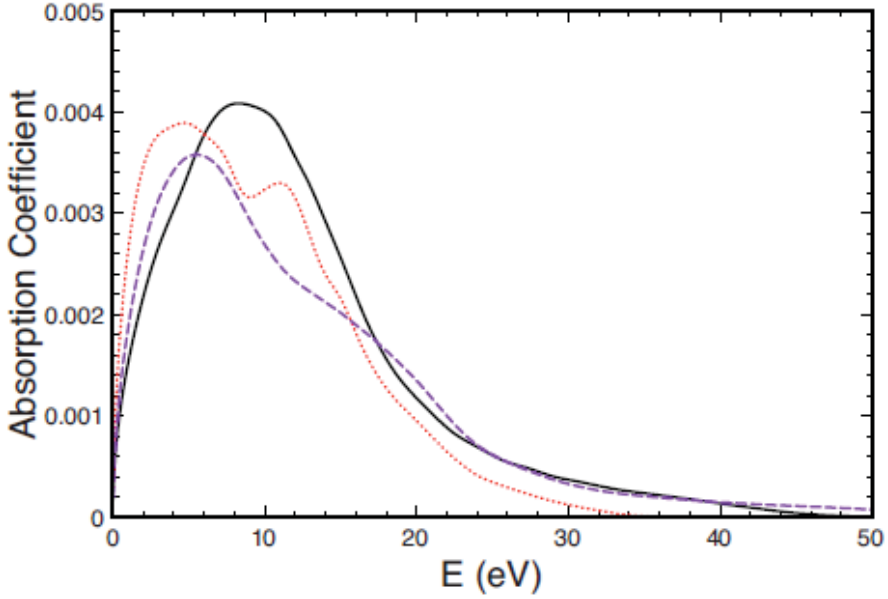


FIG. 3. (Color online) Absorption coefficient for LiH in a volume of 1824 Å^3 and 1.0 eV. Mixture [black (solid)], density matching [red (dot)], and pressure matching [violet (dash)].

1. Mixing in QMD(N_{Li}=N_H)
2. Density matching:
   V_{LiH} =V_H=V_{Li}
   P_{LiH}=P_H+P_{li}
3. Pressure matching:
   V_{LiH} = V_H+V_{Li}
   P_{LiH} = P_H=P_{Li}

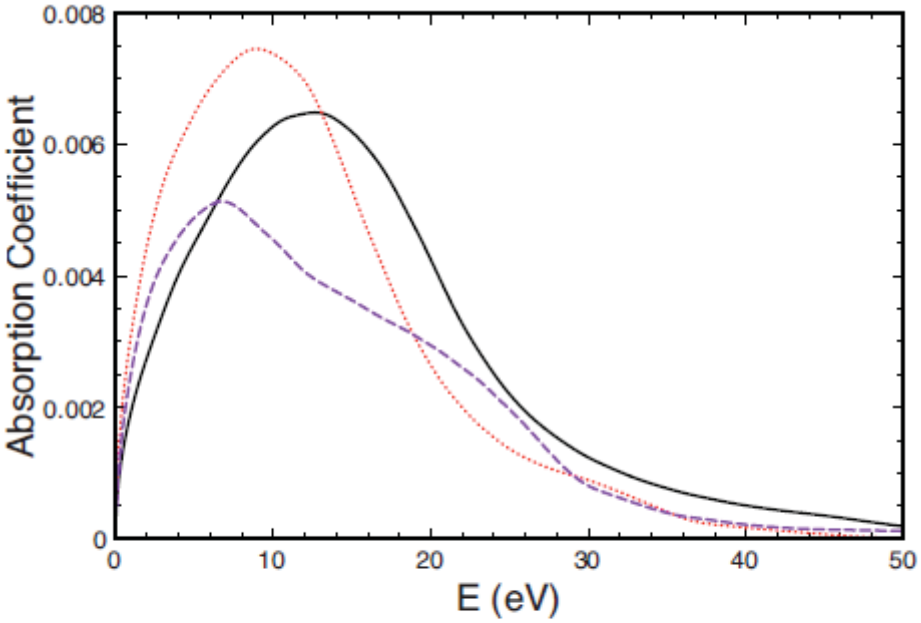
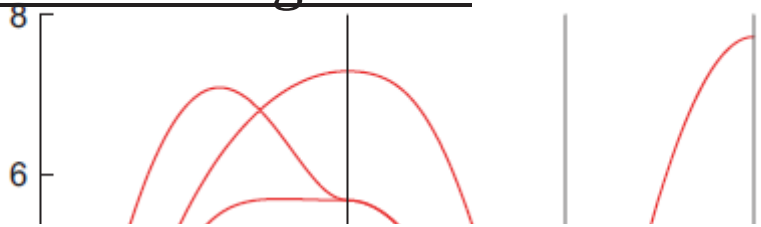
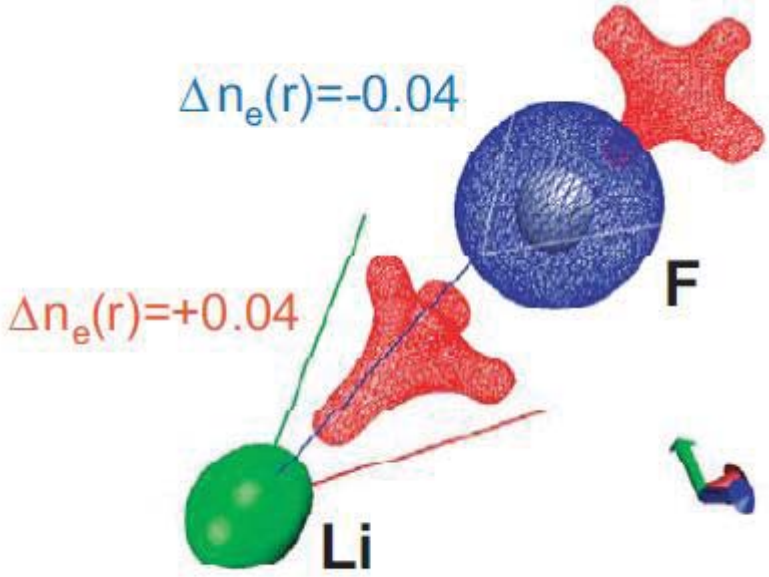


FIG. 5. (Color online) Absorption coefficient for LiH in a volume of 912 Å^3 and 1.0 eV. Mixture [black (solid)], density matching [red (dot)], and pressure matching [violet (dash)].

V.V. Stegailov , Contrib. Plasma Phys. 50, No. 1, 31 – 34 (2010)

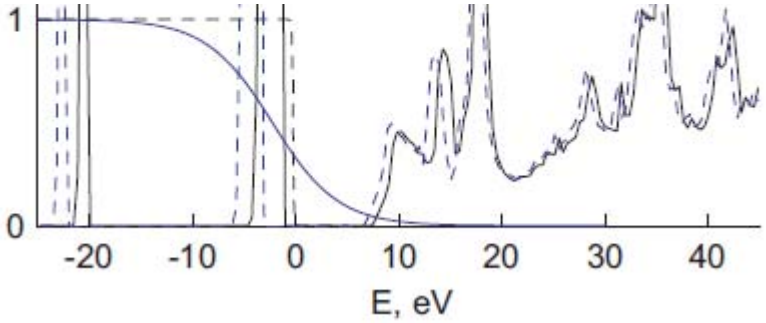
Different type of consideration for mixturing atoms





Another mixing model

Fig. 2 The unit cell of the LiF fcc lattice is shown (color online). The wireframe surfaces show the surfaces of the constant value for the difference in the electron density at different electronic temperatures $\Delta n_e = n_e(r)|_{3.2eV} - ne(r)|_{0.0eV}$: $\Delta n_e = -0.04$ (a spherical surface around the F atom) and $\Delta n_e = +0.04$ (two star-like surfaces in between Li and F).

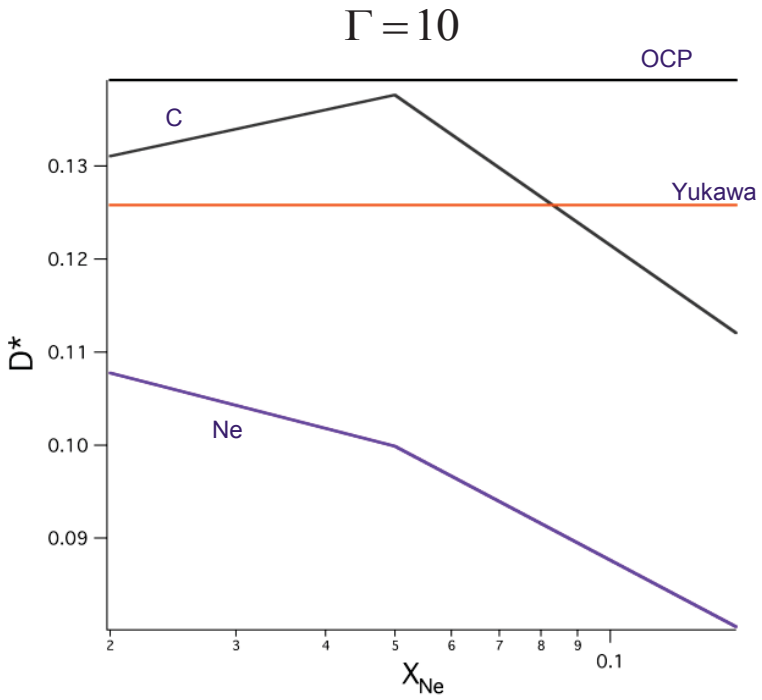


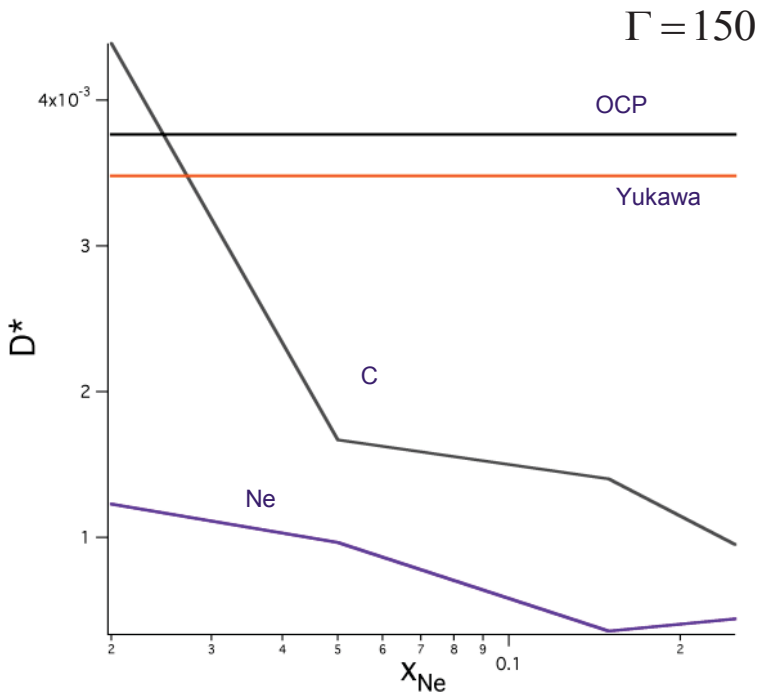
electron temperatures: Te = 2.0 (solid lines) and Te = 3.2eV (dashed lines).

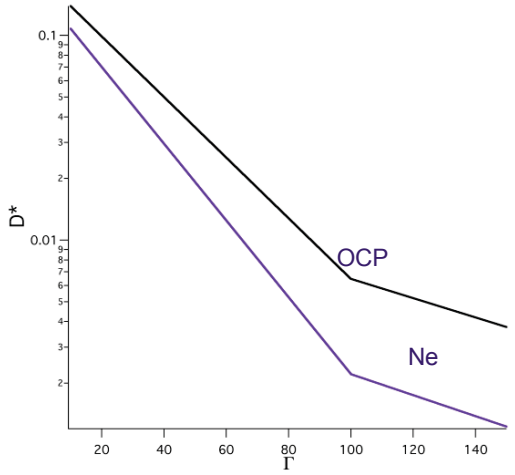
Fig. 1 The electron density of states for the fcc LiF crystal at different electron temperatures: $T_e = 0$ (solid line) and $T_e = 3.2\,\mathrm{eV}$ (dashed line). The corresponding Fermi-Dirac distributions of occupancies are shown as well.

H. Ohta and S. Hamaguchi, Phys. of Plasmas, vol.7-11 (2000)

Impurity treatment







Viscosity and diffusion constants

Transport Coefficients Obtained Via Kubo-Green Relations

$$\overline{D_{\alpha\beta}} = \frac{Q}{3Nx_\alpha x_\beta}\int_0^t \langle \mathrm{A}(0)\mathrm{A}(\mathrm{t}')\rangle dt'$$

Diffusion Coefficient: (velocity autocorrelation function)

$$D_a{}^{(R)} = \frac{1}{6t}\langle |R_{\alpha i}(t) - R_{\alpha i}(0)|^2 \rangle$$

or

$$D_a{}^{(V)} = \frac{1}{3}\int_0^\infty \langle V_{\alpha i}(t)\cdot V_{\alpha i}(0)\rangle dt$$

Viscosity Coefficient: (stress-tensor autocorrelation function)

$$\bar{\eta}(\mathrm{t}) = \frac{V}{k_B T}\int_0^t \langle P_{12}(0)P_{12}(t')\rangle dt'$$

By using MD or QMD results, we can predict viscosity and diffusion consta

Michael S. Murillo, High Energy Density Physics 4 (2008) 49~57

Yukawa Model

Potential energy is scaled by v(r) =Tu(r) $u(r) = \frac{\Gamma}{r} e^{-\kappa r}$

κ: inverse screening length

Γ: Coulomb coupling coefficient=Q^2/aT

($a= (3/4\pi n)^{1/3}$)

Characteristic Viscosity:

$$\eta_0 = \sqrt{3}\omega_E M n a^2 \quad \omega_E(k): \text{Einstein frequency}$$

Viscosity: $\frac{\eta}{\eta_0} = 0.0051\frac{\Gamma_m}{\Gamma} + 0.374\frac{\Gamma}{\Gamma_m} + 0.022$ <= coefficients from MD

Useful formula:

$$\Gamma_m(\kappa) = 171.8 + 82.8\left(e^{0.565\kappa^{1.38}} - 1\right)$$

$$\sqrt{3}\omega_E(\kappa) = \omega_i e^{-0.2\kappa^{1.62}}$$

$$\omega_i = \sqrt{4\pi n Q^2/M}$$

Michael S. Murillo, High Energy Density Physics 4 (2008) 49~57

Good agreement for material at T~Tm

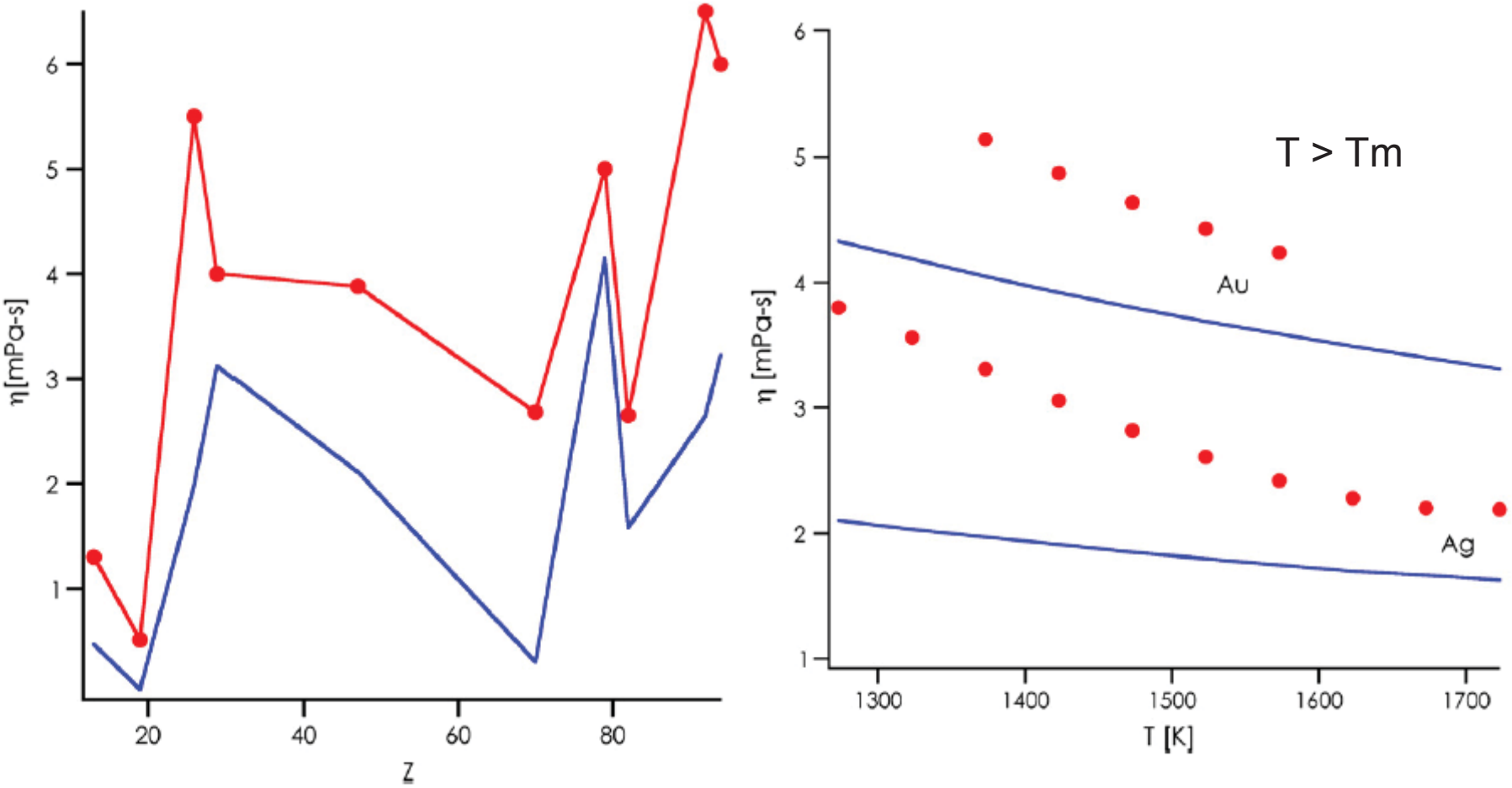


Fig. 1. The viscosity of various elements (Al, K, Fe, Cu, Ag, Yb, Au, Pb, U, and Pu) at their melting temperatures is shown. Experimental data are shown in red and predictions of the YVM model are shown in blue. (For interpretation of colors in this article, the reader is referred to the web version of the article.)

Larger fluctuation at $T<10^4K$

Good agreement from $T>10^4K$

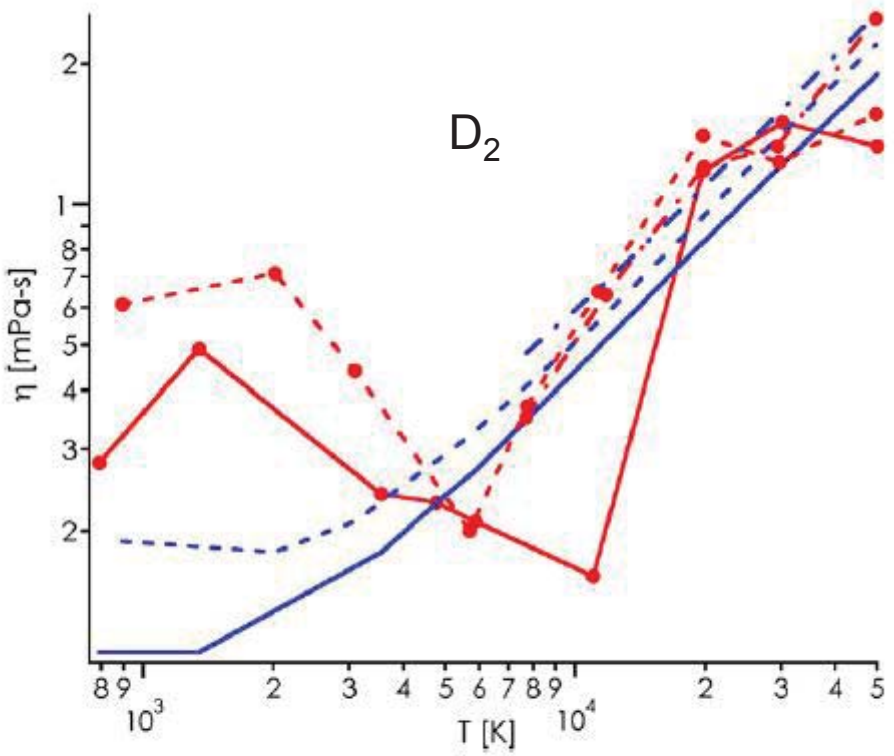


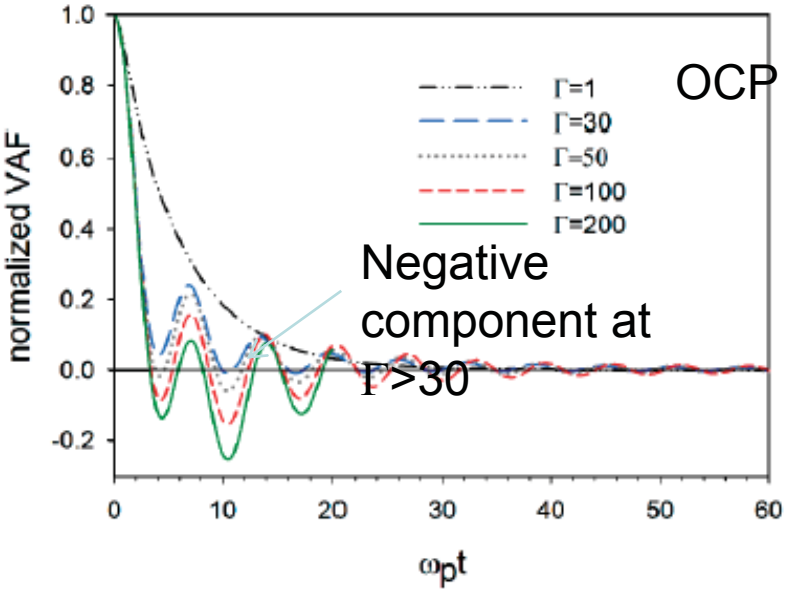
Fig. 3. The data from Table 1, for dense deuterium, are shown. The MD (red) and YVM (blue) viscosity predictions are shown versus temperature for the three densities $\rho = 0.665$ (solid), $\rho = 1.0$ g/cm^3 (long dash), and $\rho = 1.0$ g/cm^3 (dash-dot). (For interpretation of colors in this article, the reader is referred to the web version of the article.)

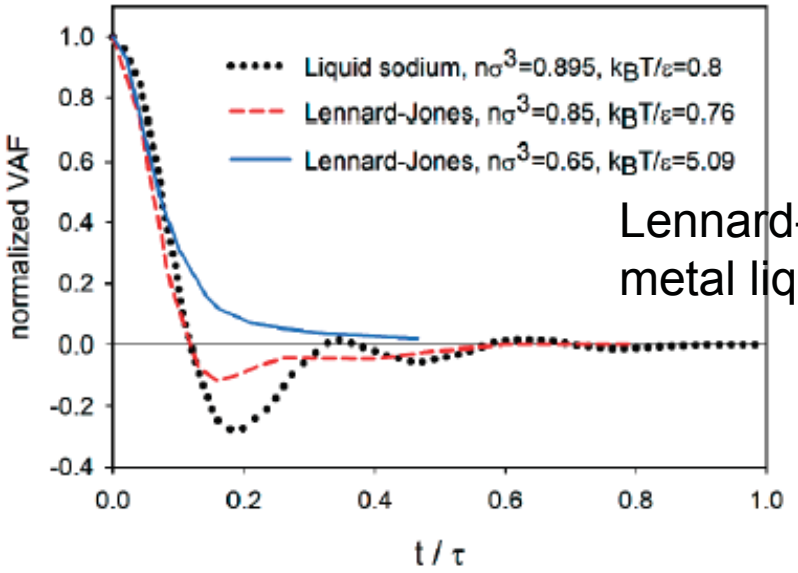
Molecular dissociation ?

Jerome Daligault, PRL **96,** 065003 (2006)

Model is good at $\Gamma > 50$

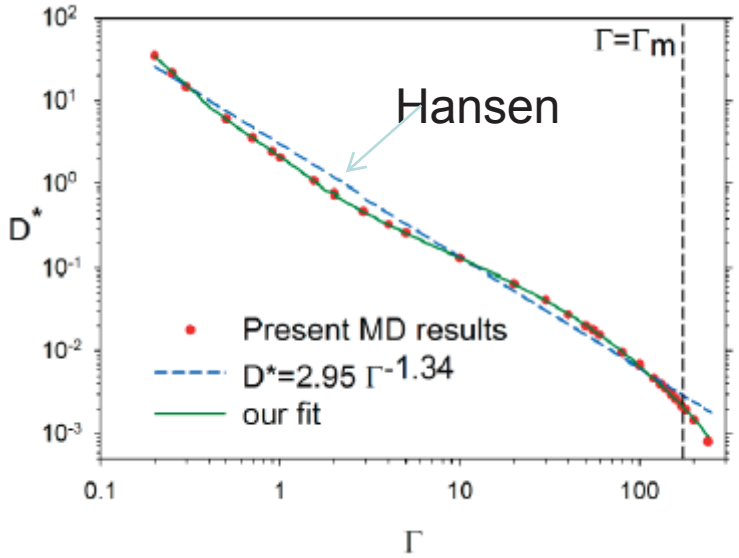
velocity autocorrelation function



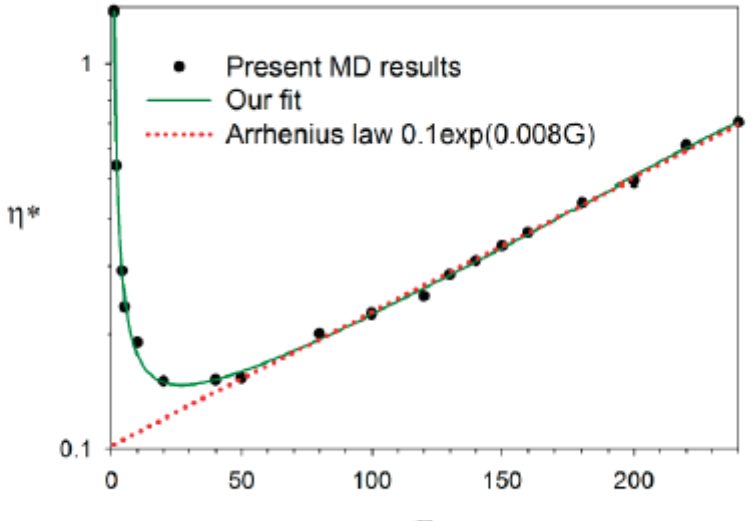


Lennard-Jones metal liquids

Self diffusion *D*



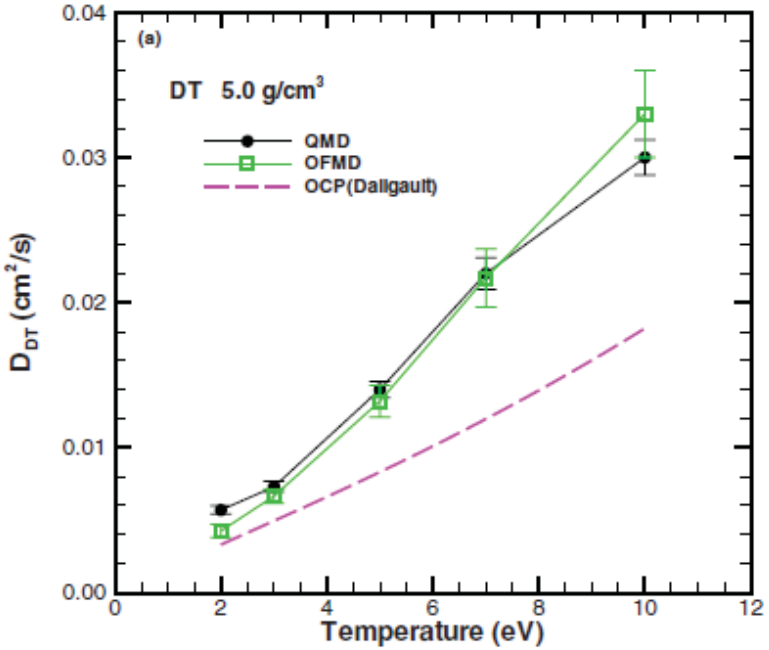
Shear viscosity

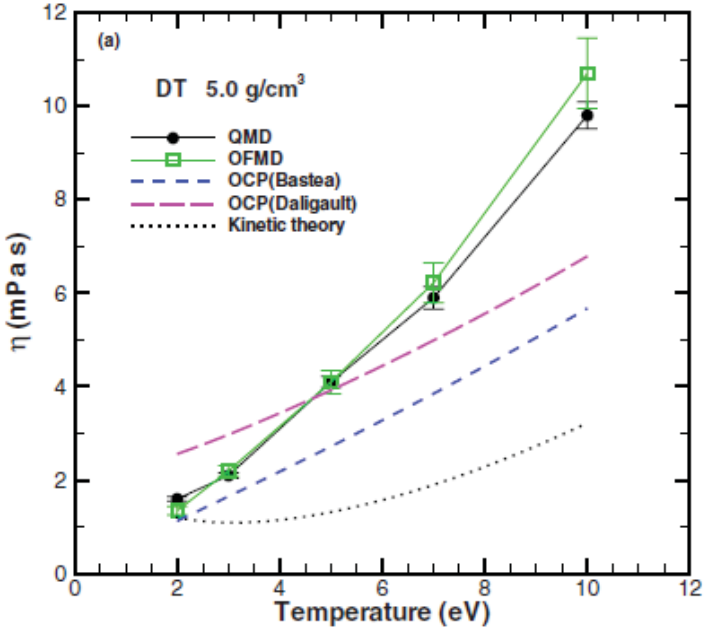


"Cage" effect formed by immediate neighbo

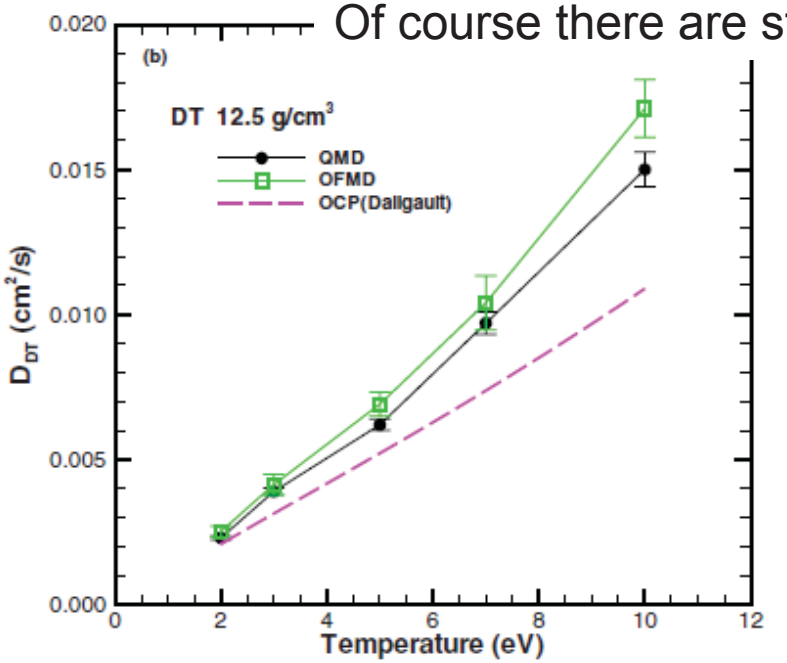
J. D. Kress, James S. Cohen, D. A. Horner, F. Lambert, and L. A. Collins, PHYSICAL REVIEW E **82**, 03640

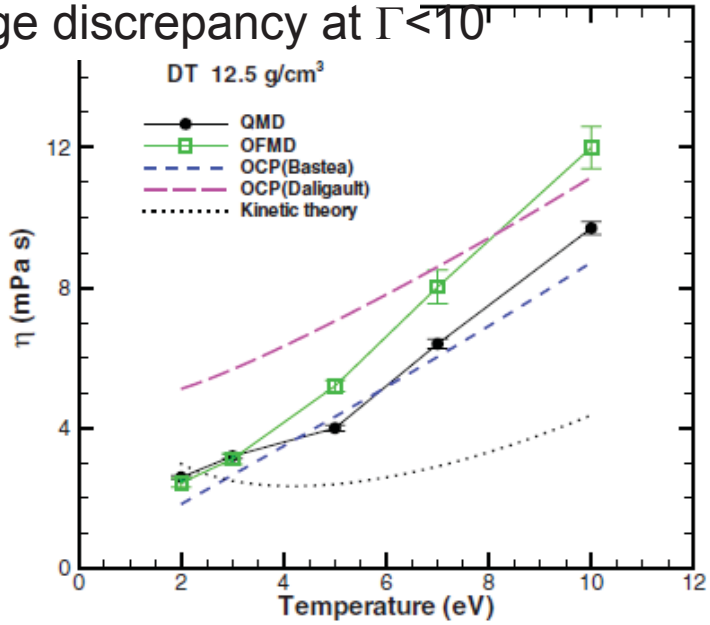
$\Gamma<10$





Of course there are still large discrepancy at $\Gamma<10$





summary

- WDM physics investigation with basic Physics Textbook.
- QMD calculation is a strong tool for prediction of WDM phenomena.
- Every theoretical modeling should be checked by reliable experiments.
- There are many application such as laser machining, peening, reactor wall, re-entry vehicles in addition with brand new application like high energy science and applications.

Michael S. Murillo, et al., LA-UR-05-0111

A Warm Dense Matter Parameter ?

We can define a "WDM parameter" as:

$$W \equiv \exp\left[-(1-\Gamma)^2\right] \cdot \exp\left[-(1-\Phi)^2\right]$$

For a real material, we need to consider ioniza

$$\bar{Z}(\rho,T)$$

$$n_e^f = \bar{Z}(\rho,T)\frac{\rho}{M_i}$$

$$E_F = \frac{\hbar^2\left(3\pi^2 n_e^f\right)^{2/3}}{2m_e}$$

$$\Gamma_{ee} = \frac{e^2}{a_e\sqrt{T^2+E_F^2}}$$

To estimate *W*, use a simple Thomas-Fermi model for $Z(\rho,T)$.