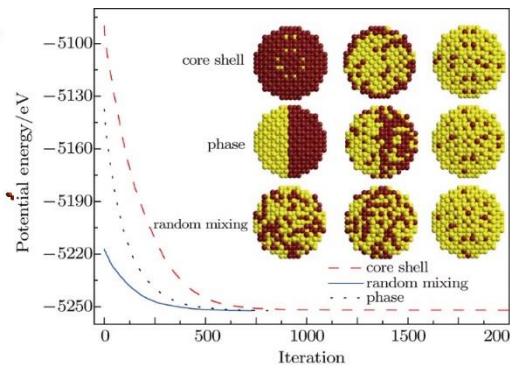
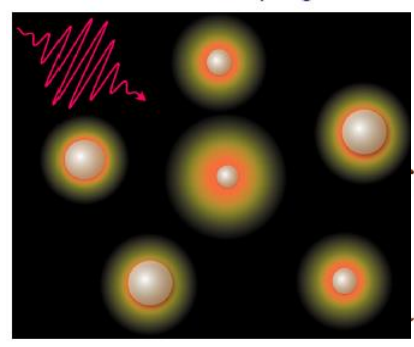
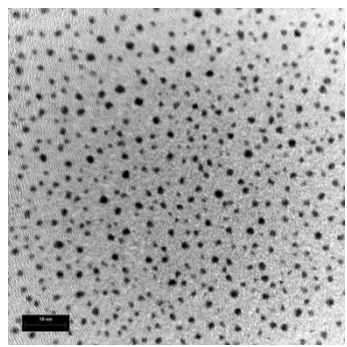
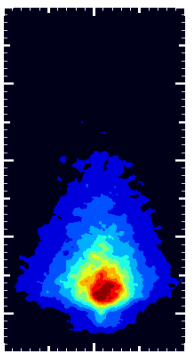


Molecular Dynamics Simulations of Laser-Matter Interactions

Tatiana ITINA

Laboratoire Hubert Curien, UMR CNRS 5516, Saint-Etienne, France



From laser plume with nanoparticles to nanohybrides...

Molecular Dynamics (MD)

- **Newton or Hamilton equations**

$$m d^2r/dt^2 = F = -\nabla U,$$

- **Construct a 'system'** (input: positions, velocities et chemical elements, potentials, interaction potentials, etc...)

- **Choosing parameters**

Cohesive energies, densities, elastic and thermal properties..

- **Integration**

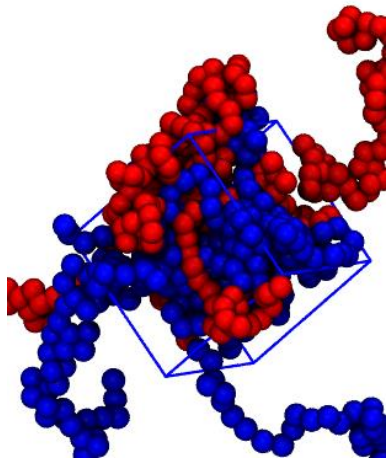
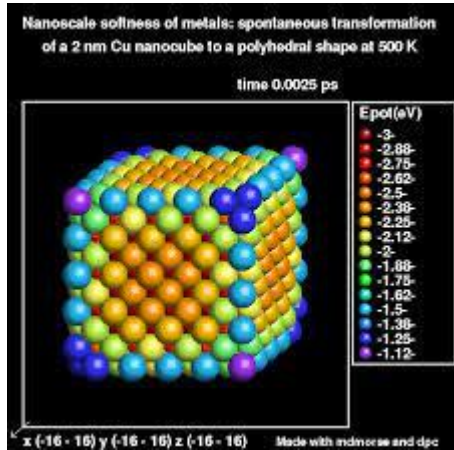
$$v(t+\delta t) = v(t) + F(t)*\delta t/m$$

$$r(t+\delta t) = r(t) + v(t)*\delta t$$

- **Output**

temperature, pressure, composition,
energy & distributions ,
etc...

Molecular Dynamics (DM): solids, liquids, phase transitions

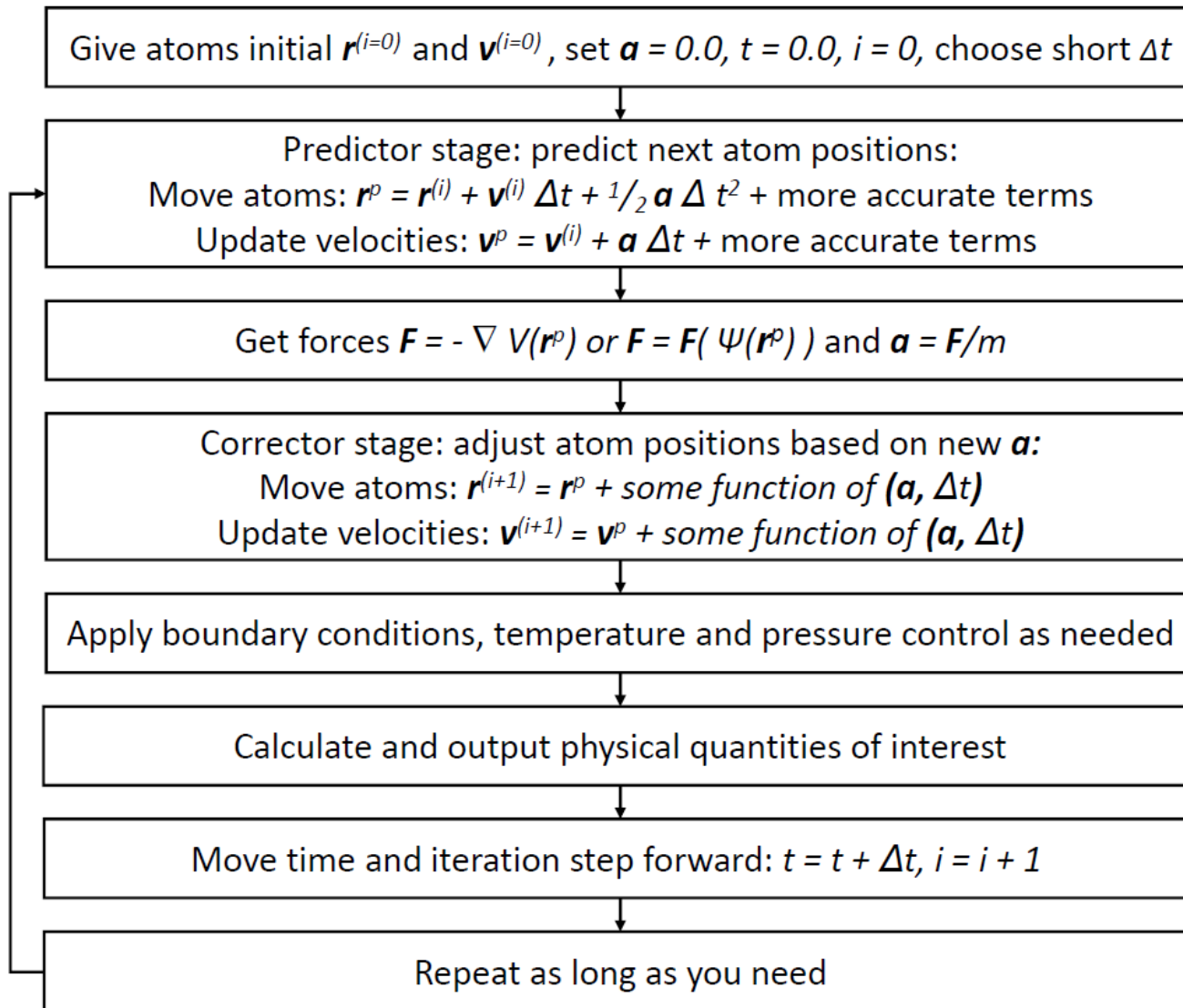


- Construct a sample: set initial atom's positions, types, masses
- Define boundary conditions
- Define interaction potential
- Often need to fit parameters to properties such as *cohesive energies, densities, elastic properties,...*
- Give initial velocities according to T
(often need to heat and cool the sample – quenching procedure)

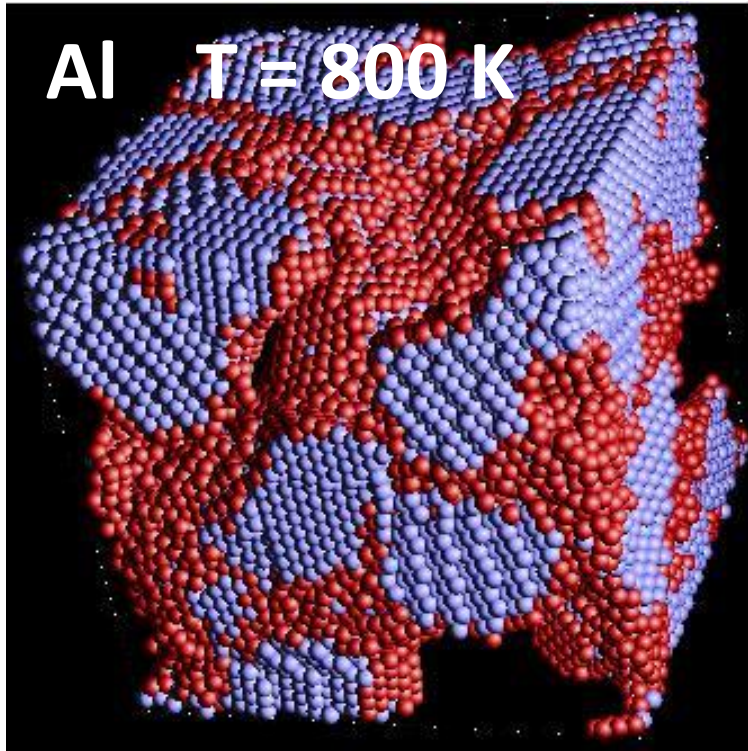
- Fix the dynamics – how T (or, E,N,V, P) will change
- Choose time step
- Integrate Newton's or Hamilton's equations of motion.
 $md^2r/dt^2 = F = -\nabla U$, where U is the potential
- Integration of the differential equations
 $v(t+\delta t) = v(t) + F(t)*\delta t/m$
 $r(t+\delta t) = r(t) + v(t)*\delta t$

- Think about yields: snapshots, temperature, pressure, energy & angular distributions, etc...

Simplified schematic of the molecular dynamics algorithm



Molecular Dynamics (DM): integration



K. Kadau & M. Kreth



$$m_k \ddot{\vec{x}}_k(t) = F_k(\vec{x}(t))$$

Integration : Verlet

$$\vec{x}(t + \Delta t) = \vec{x}(t) + \vec{v}(t) \Delta t + \frac{1}{2} \vec{a}(t) \Delta t^2$$
$$\vec{v}(t + \Delta t) = \vec{v}(t) + \frac{\vec{a}(t) + \vec{a}(t + \Delta t)}{2} \Delta t$$

Potentiels, par exemple: EAM

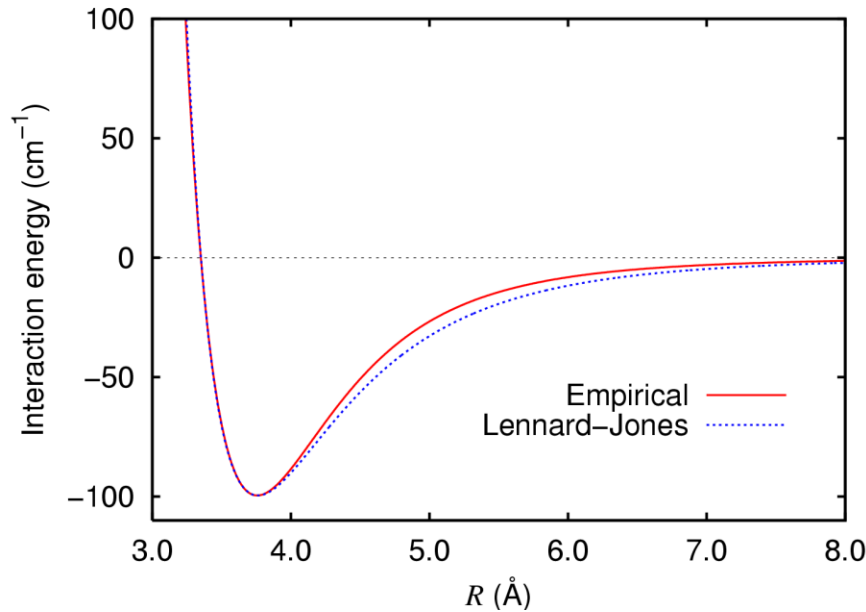
$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

MD: interaction potentials

$$m d^2 r / dt^2 = F = -\nabla U$$

Lennard-Jones (Ar)

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right],$$



- Morse (molecules)

$$V(r) - D_e = D_e (e^{2a(r_e - r)} - 2e^{a(r_e - r)})$$

- Stillinger-Weber (Si, 3 cors)

$$V = \frac{1}{2} \sum_{ij} \phi(r_{ij}) + \sum_{ijk} g(r_{ij})g(r_{ik}) \left(\cos \theta_{jik} + \frac{1}{3} \right)^2$$

- Embedded atom (EAM)

- Terstoff (Si, GaAs, Ge), Brenner (C, HC), Terstoff-Brenner

- Impirical

-

Input / Output

Atomic / molecular size

Atomic / molecular mass

Crystal structure

Interaction potentials

Time step

Dynamics

Boundary conditions

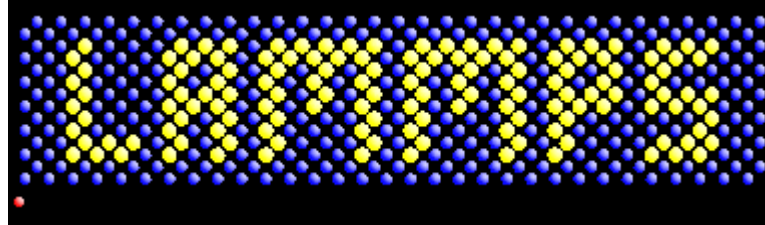
Species distributions and velocities

Energies : E_p , E_k , E_{tot} , etc..

Shapes, snapshots, movies

LAMMPS Molecular Dynamics Simulator

LAMP is a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul -- www.dictionary.com



LAMMPS is a classical molecular dynamics (MD) code

The LAMMPS Homepage has moved to <https://www.lammps.org>

2021 Virtual LAMMPS Workshop and Symposium, week of Aug 9th, hosted by Temple University

See: <https://www.lammps.org/tutorials>

LAMMPS Molecular Dynamics : examples

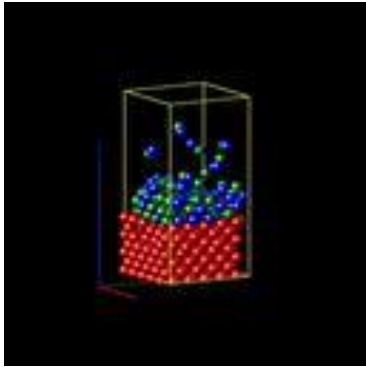
[examples/README](#) has one-line descriptions of 30 examples

Quick runs (2d) and visually appealing:

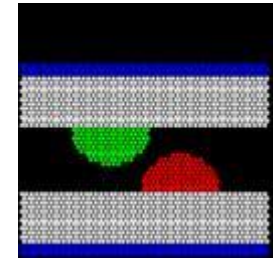
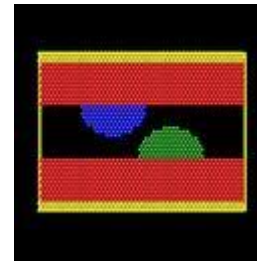
- [colloid](#): colloidal particles in solution
- [crack](#): crack propagation
- [flow](#): Couette and Poiseuille flow in a channel
- [friction](#): frictional contact of spherical asperities
- [indent](#): spherical indenter into solid
- [micelle](#): self-assembly of small lipid-like molecules
- [nemd](#): continuous non-equilibrium shear of LJ liquid
- [obstacle](#): flow around two voids in a channel
- [pour](#): pouring of granular particles into a box
- [shear](#): sideways shear of solid, with and without a void

<https://www.lammps.org/movies.html>

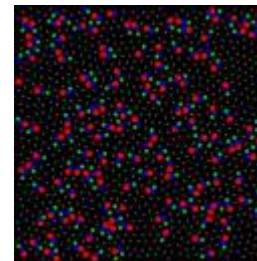
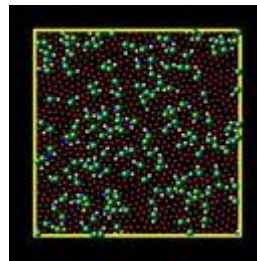
Deposition of atoms and molecules



Friction between 2 surfaces



Micelle self-assembly



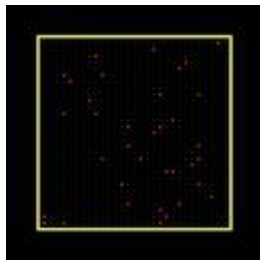
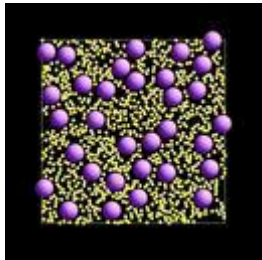
and much more....

Colloids in a solvent

for this problem from the examples directories.

Colloids of diameter 5 are put in a background solvent of Lennard-Jones particles (diameter 1). The big-big and big-small particle interactions are calculated via the [pair_style colloid](#) potential in a 2d system. The system is initialized very dilute and then run at constant pressure. The simulation box in the first movie thus shrinks and oscillates initially.

In the second movie, made with the [dump image](#) command, the displayed box size is scaled to the same value for every frame, so it appears that the particles [grow](#) in size as the box shrinks.



```
# Big colloid particles and small LJ particles
```

```
units                               lj
atom_style                           sphere
dimension                             2
lattice                               sq 0.01
region                               box block 0 30 0 30 -0.5 0.5
create_box                           2 box
create_atoms                          1 box
```

```
set                                   group all type/fraction 2 0.96 23984
```

```
set                                   type 1 mass 9
set                                   type 2 mass 1
velocity                             all create 1.44 87287 loop geom
```

```
# multi neighbor and comm for efficiency
```

```
neighbor                             1 multi
neigh_modify                          delay 0
comm_modify                           mode multi
```

```
# colloid potential
```

```
pair_style                            colloid 12.5
pair_coeff                             1 1 1.0 1.0 5.0 5.0 12.5
pair_coeff                             1 2 5.0 1.0 5.0 0.0 7.0
pair_coeff                             2 2 10.0 1.0 0.0 0.0 2.5
```

```
fix                                    1 all npt temp 2.0 2.0 1.0 iso 0.0 1.0 10.0 drag 1.0
&
```

```
fix                                    mtk no pchain 0 tchain 1
2 all enforce2d
```

```
#dump                                  1 all atom 1000 dump.colloid
```

```
#dump                                  2 all image 1000 image.*.jpg type type &
#                                       zoom 1.5 center d 0.5 0.5 0.5
#dump_modify                           2 pad 5 adiam 1 5.0 adiam 2 1.5
```

```
#dump                                  3 all movie 1000 movie.mpg type type &
#                                       zoom 1.5 center d 0.5 0.5 0.5
#dump_modify                           3 pad 5 adiam 1 5.0 adiam 2 1.5
```

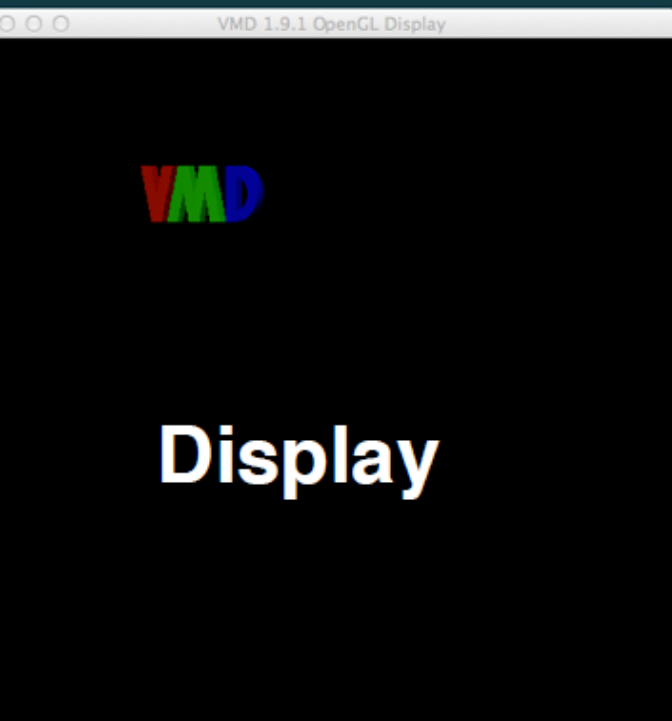
```
thermo_style                          custom step temp epair etotal press vol
thermo                                  1000
```

```
timestep                               0.005
run                                     50000
```

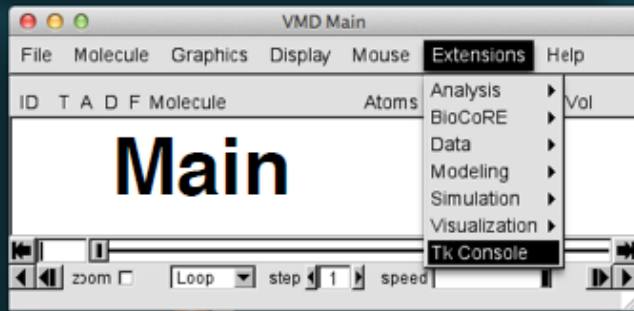
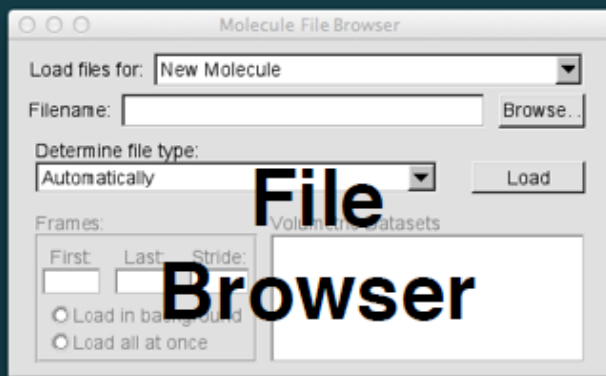
LAMMPS : scripting and visualization

VMD Features

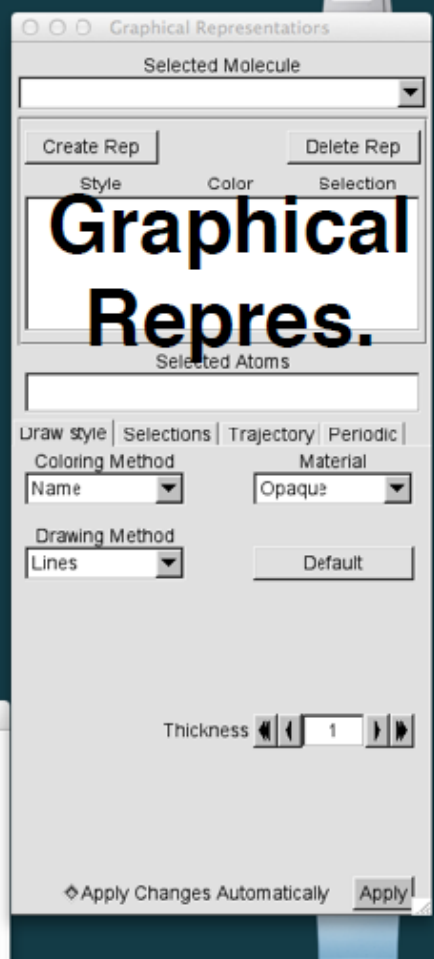
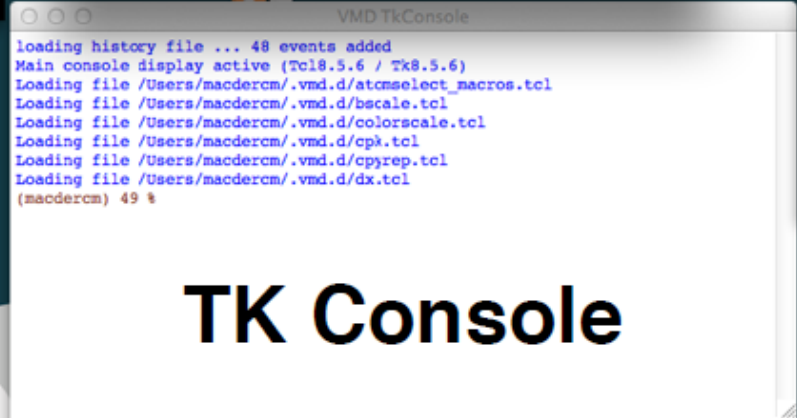
- Support for all major computer platforms
- Support for multicore processors
- Support for GPU accelerated computation
- No limits on the number of molecules, atoms, residues or number of trajectory frames, **except available memory**
- Many molecular rendering and coloring methods
- Extensive atom selection syntax for choosing subsets of atoms for display (includes boolean operators, regular expressions, and more)
- Support for over 60 molecular file formats and data types through an extensive library of built-in file reader/writer plugins and translators



Display



TK Console



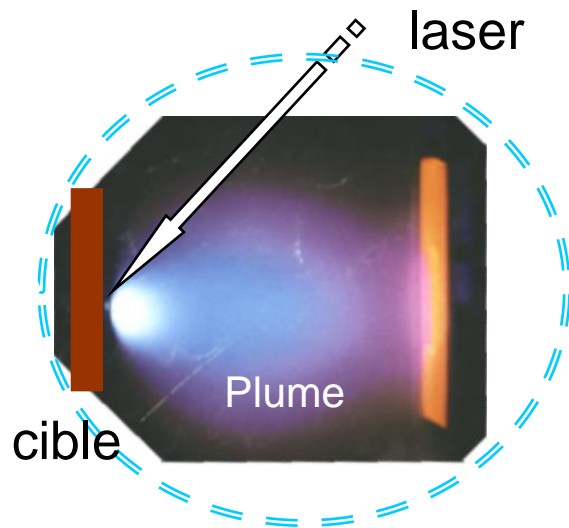
vmd

LAMMPS : Python interface

The image displays the LAMMPS Python interface with four main components:

- Terminal:** Shows the simulation progress with columns for Step, Temp, E_pair, E_sml, TotErg, and Press. It includes performance metrics like 'Loop time of 0.0438259 on 1 proc for 100 steps with 900 atoms' and a summary of time spent on various tasks.
- Graph 1:** A plot titled 'Therm_1.log' showing Temperature vs. Timestep. The temperature starts at approximately 1.0, jumps to 2.5 at timestep 400, and then drops to 0.0 at timestep 800.
- LAMMPS GUI:** A control panel with buttons for Run, Stop, and Quit, and a Temperature input field set to 0.1.
- Visualization:** A 'Playview' window showing a 3D visualization of a dense packing of atoms, represented as small spheres.

Laser plasmas



Laser interaction with a solid or a liquid surface

Energy propagation, reflection and absorption

Heating, pressure wave formation, phase transitions

Ablation, plasma plume expansion, reactions, clustering, etc...

Often multi-pulse irradiation is used.

Nanosecond laser

Combined Hydrodynamic- Monte Carlo Modelling

$t < t_0$ **Continuos hydrodynamics (LP)**

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{W}) = 0$$

$$\frac{\partial \rho U}{\partial t} + \text{div}(\rho U \vec{W}) + \frac{\partial P}{\partial z} = 0$$

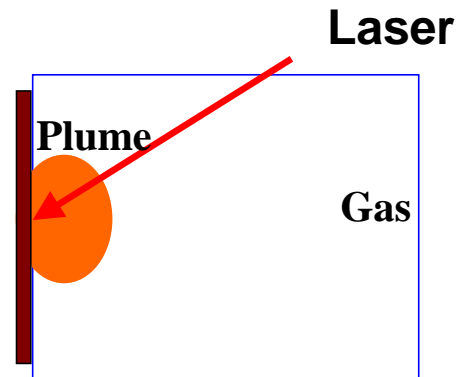
$$\frac{\partial \rho V}{\partial t} + \text{div}(\rho V \vec{W}) + \frac{\partial P}{\partial r} = 0$$

$$\frac{\partial \rho E_a}{\partial t} + \text{div}(\rho E_a \vec{W}) + \text{div}(P_a \vec{W}) = Q_{ei} + Q_{ea}$$

$$\frac{\partial \rho E}{\partial t} + \text{div}(\rho E \vec{W}) + \text{div}(P \vec{W}) = -F$$

$$\rho(r, z, t), E(r, z, t), V(r, z, t), U(r, z, t)$$

$t > t_0$ **Direct Simulation Monte Carlo (DSMC)**

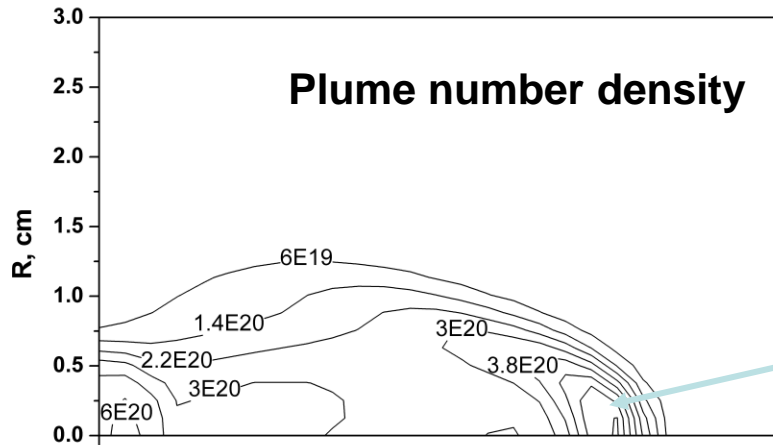


- ensemble of particles
- small cells ($l < \lambda$)

Nanosecond laser ablation in a gas

Snowplough effect

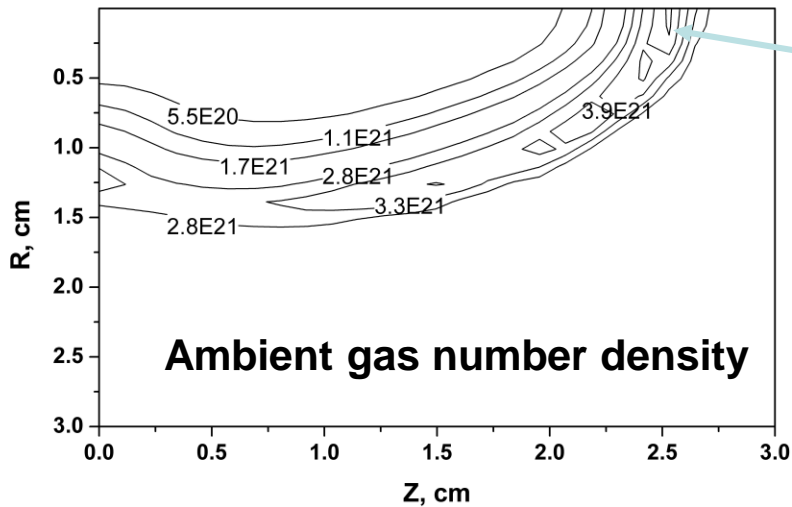
$t=2.6 \mu\text{s}$



Al in O₂

$R_0 = 1 \text{ mm}$, $P=70 \text{ Pa}$

•Plume compression



•Background gas compression

Nd:YAG (266 nm) laser, $\tau=5 \text{ ns}$,

$R_0 = 1 \text{ mm}$, $F=20 \text{ J/cm}^2$

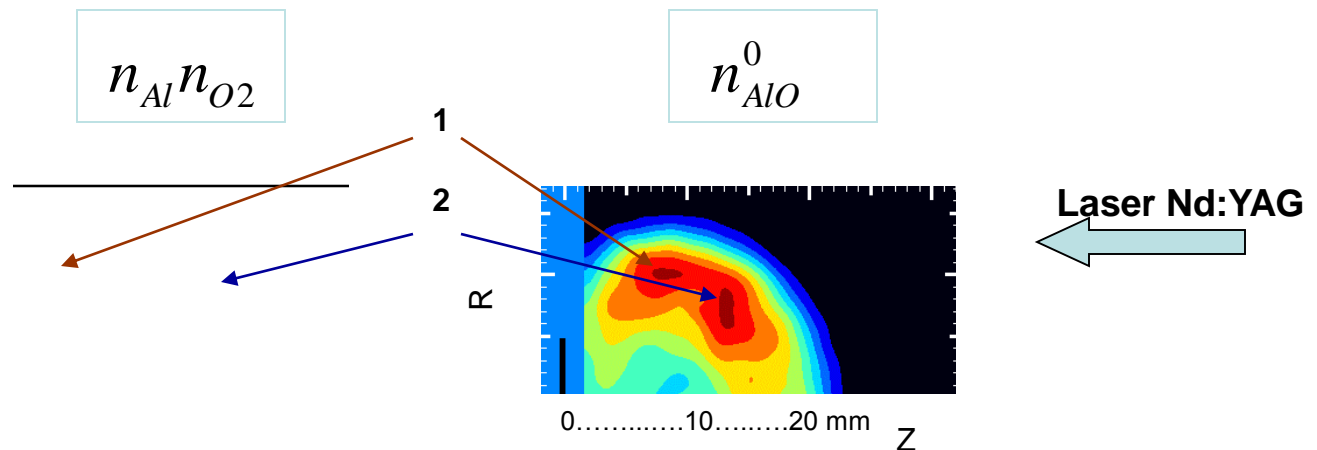
Nanosecond laser

Modeling explains reactive ablation experiments

Al in O₂, P = 13 Pa, t = 3 μs

LP-DSMC calculations

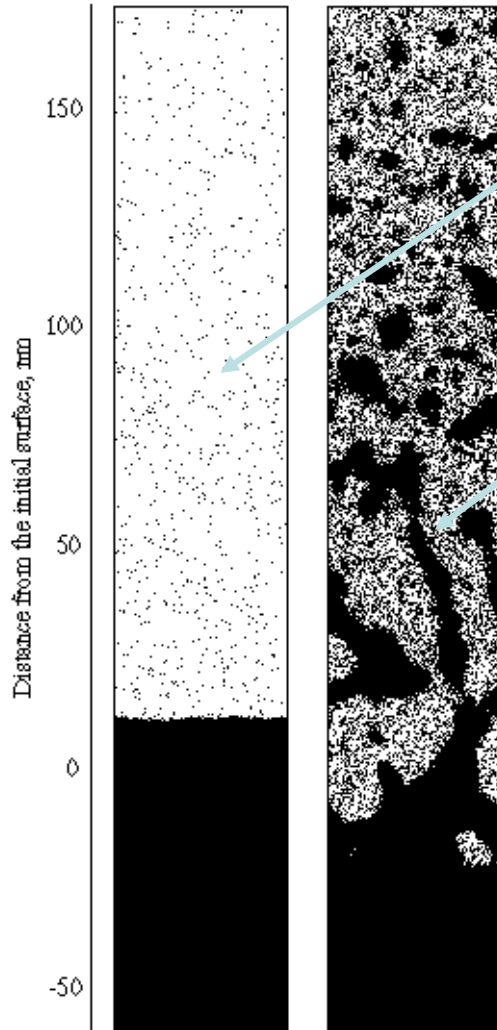
LIF experiments



maxima are due to mixing
at the locations of the back (1) and radial (2) flows

MD Simulations of Picosecond Laser Ablation

Laser pico



$F < F_{th}$

Desorption: Mostly atoms, slow surface evaporation process

$F > F_{th}$

Ablation: Ejection of a mixture of gas and aggregates, rapide volume process

Non-equilibrium process, $T \rightarrow T_c$

difficult for classical modeling (continuous)

Input / Output

Atomic / molecular size

Atomic / molecular mass

Interaction potentials

Laser parameters (wavelength, pulse duration and shape, fluence, intensity)

Absorption / excitation coefficient

Boundary conditions

Atomic / molecular ejection

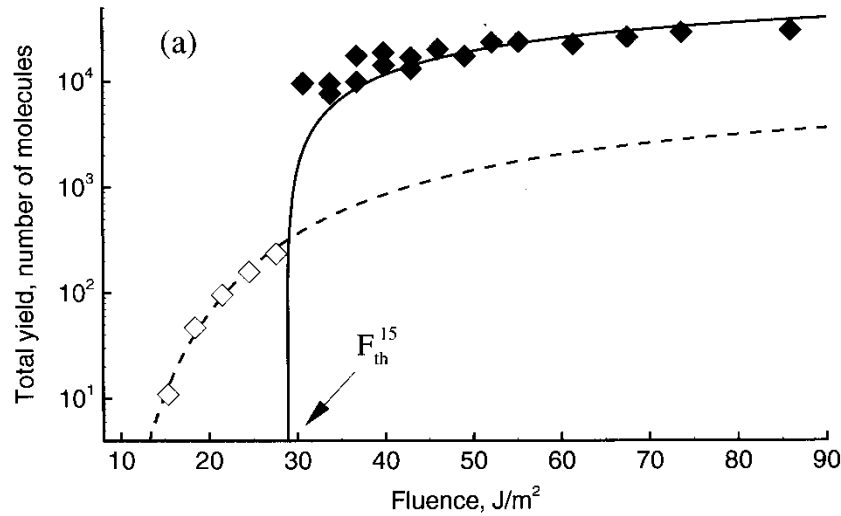
Concentration of species / aggregates, and their distributions

Ablated depth

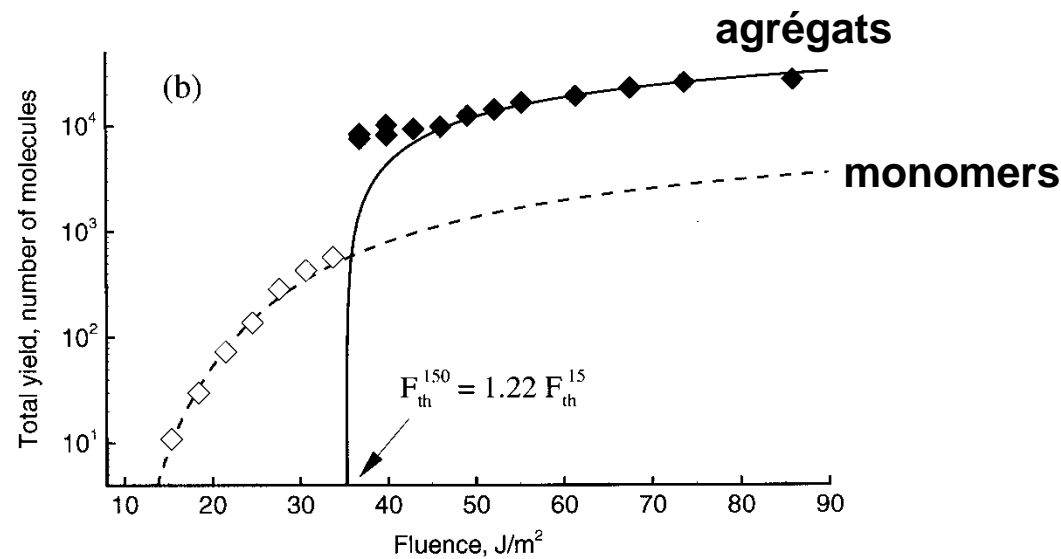
Shape of craters

Potential and kinetic energies

Confinement mécanique vs thermique



Confinement mécanique
pulse ~15 ps



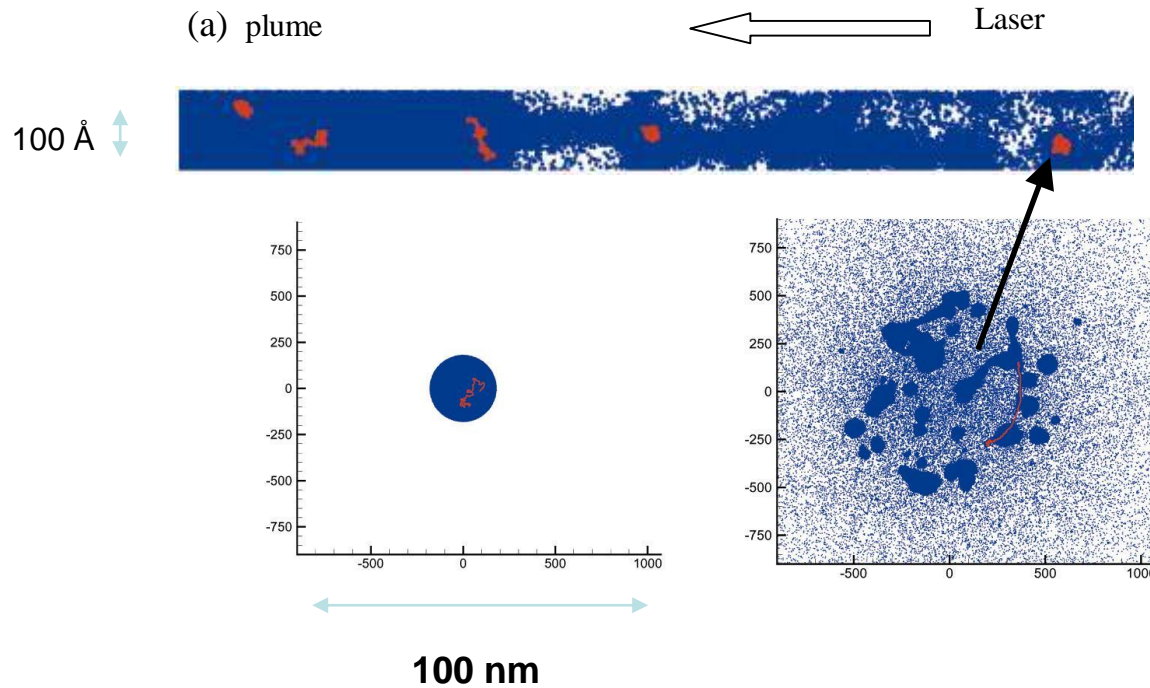
Confinement thermique
pulse 150 ps

En femto:
Temps de relaxation e-i

Matrice moléculaire

Zhigilei et al. Appl. Phys. A, 69, S75-S80 (1999)

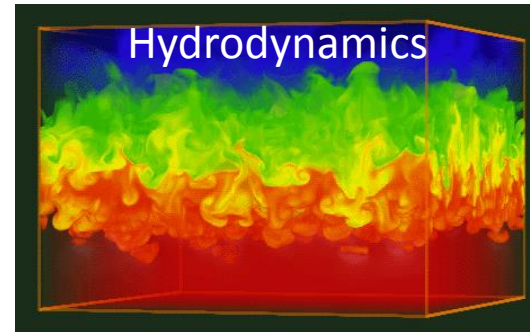
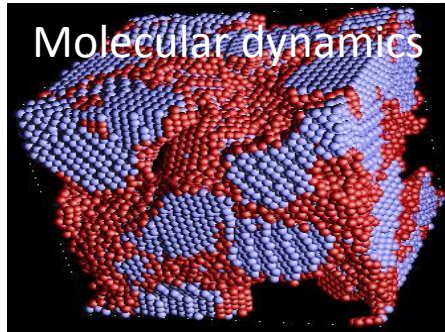
Decomposition of the ablated material after the absorption of laser radiation



**t = 300 ps after the
beginning of the laser pulse**
 $\tau = 15$ ps
e=0.6 eV per molecule

Itina&Zhigilei&Garrison

MD vs CFD



$V < 1 \mu\text{m}^3$; $t \sim 1 \text{ ns}$

Dynamics

Interaction potential

Ionization?

Real temporal and spatial scales

LTE?

Nucleation, surface effects?

Equation of state (EOS)

Povarnitsyn et al. PRB 2015

Ultra-short laser ablation of metals

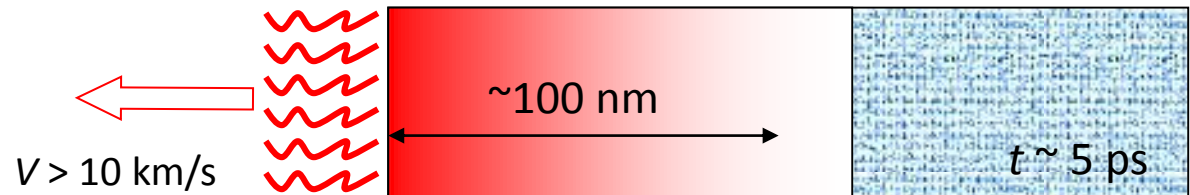
1. Pulse duration $\tau \sim 100$ fs



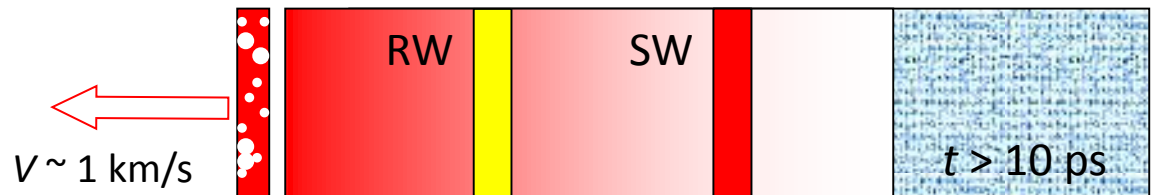
2. Absorption, e-excitation



3. Electron-phonon/ion coupling, thermal conductivity



4. Evaporation, shock waves, rarefaction waves



5. Phase explosion, material decomposition



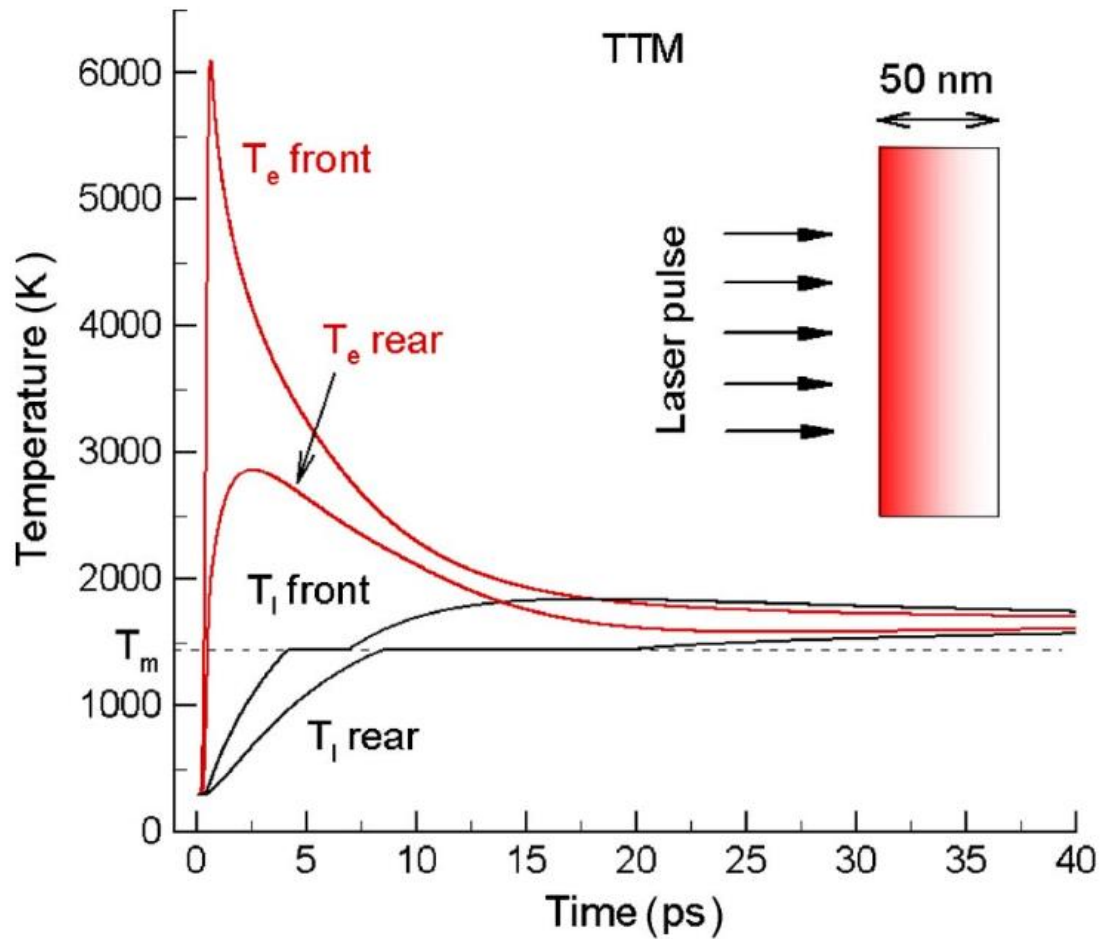
Two-temperature model (TTM)

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \nabla [K_e(T_e) \nabla T_e] - G(T_e - T_l) + S(z, t),$$

$$C_l(T_l) \frac{\partial T_l}{\partial t} = \nabla [K_l(T_l) \nabla T_l] + G(T_e - T_l),$$

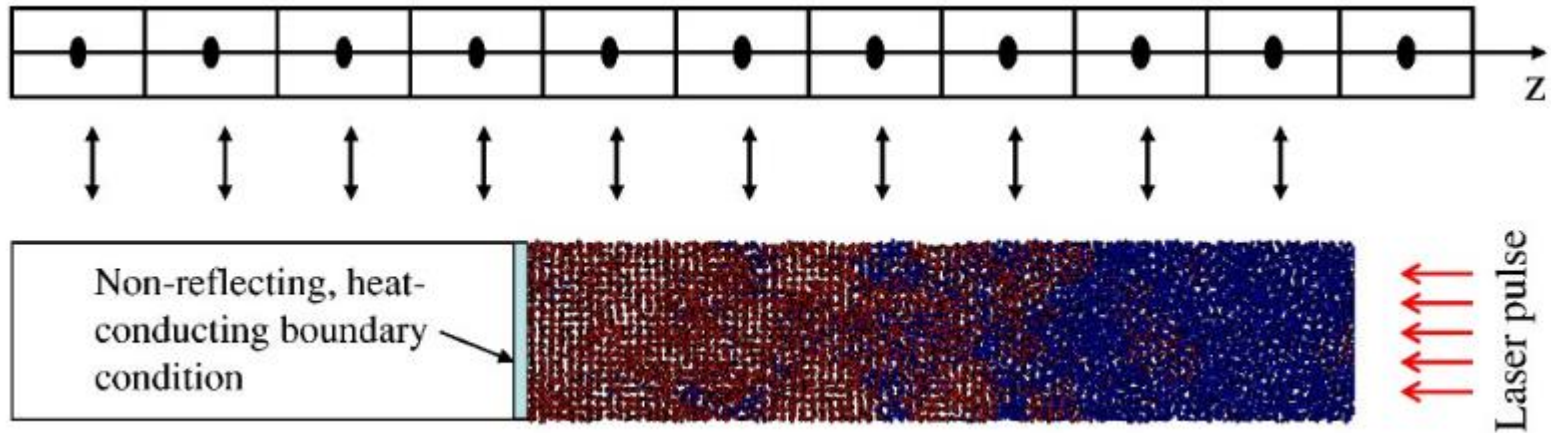
M.I. Kaganov, I.M. Lifshitz, and L.V. Tanatarov, Sov. Phys. JETP 4, 173 (1957)

Two-temperature model (TTM)



Molecular Dynamics + TTM (TTM-MD)

Électrons de conduction



$$C_e(T_e) \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial z} \left(K_e(T_e) \frac{\partial T_e}{\partial z} \right) - G(T_e - T_l) + S(z, t), \quad \text{TTM}$$

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i + \xi m_i \mathbf{v}_i^T, \quad \text{MD} \quad \xi = \frac{1}{n} \sum_{k=1}^n G V_N (T_e^k - T_l) \bigg/ \sum_i m_i (\mathbf{v}_i^T)^2$$

Ivanov & Zhigilei, Phys. Rev. B, 68, 064114 (2003)

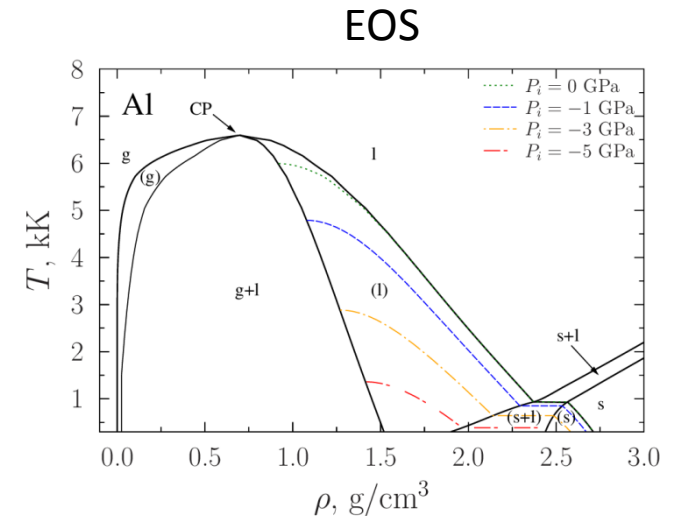
MD vs CFD

$$\frac{\partial(1/\rho)}{\partial t} - \frac{\partial u}{\partial m} = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial(P_{\text{ion}} + P_{\text{el}})}{\partial m} = 0$$

$$\frac{\partial e_{\text{ion}}}{\partial t} + P_{\text{ion}} \frac{\partial u}{\partial m} = \gamma_{ei}(T_{\text{el}} - T_{\text{io}})/\rho$$

$$\frac{\partial e_{\text{el}}}{\partial t} + P_{\text{el}} \frac{\partial u}{\partial m} = \frac{\partial}{\partial m} \left(\rho \kappa_{\text{el}} \frac{\partial T_{\text{el}}}{\partial m} \right) - \gamma_{ei}(T_{\text{el}} - T_{\text{ion}})/\rho + Q_L/\rho$$



$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i + \xi_i m_i \mathbf{v}_i^T + \mathbf{F}_i^{\text{el}} \quad \text{LAMMPS}$$

$$\frac{\partial(\rho e_{\text{el}})}{\partial t} + \frac{\partial(\rho e_{\text{el}} u)}{\partial z} + P_{\text{el}} \frac{\partial u}{\partial z} = \frac{\partial}{\partial z} \left(\kappa_{\text{el}} \frac{\partial T_{\text{el}}}{\partial z} \right) - \gamma_{ei}(T_{\text{el}} - T_{\text{ion}}) + Q_L(t, z)$$

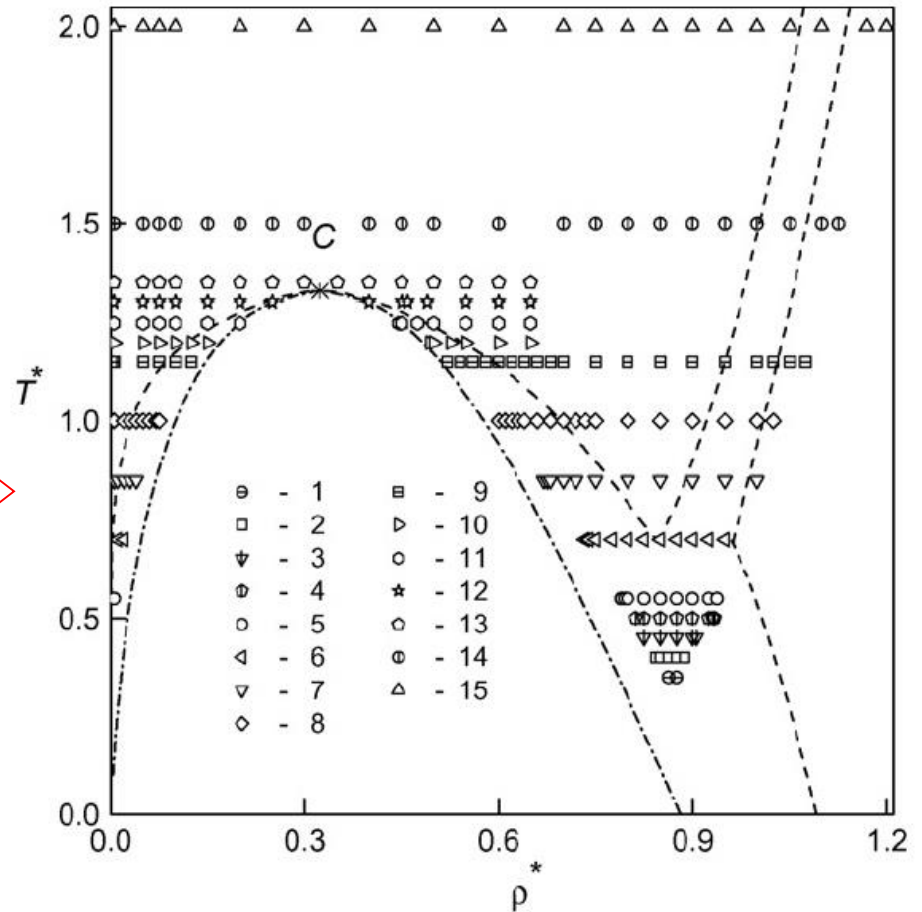
Embedded atom "EAM"

$$E_i = F_{\alpha} \left(\sum_{j \neq i} \rho_{\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

Zhakhovskii *et al.* Appl. Surf. Sci. 255 (2009)

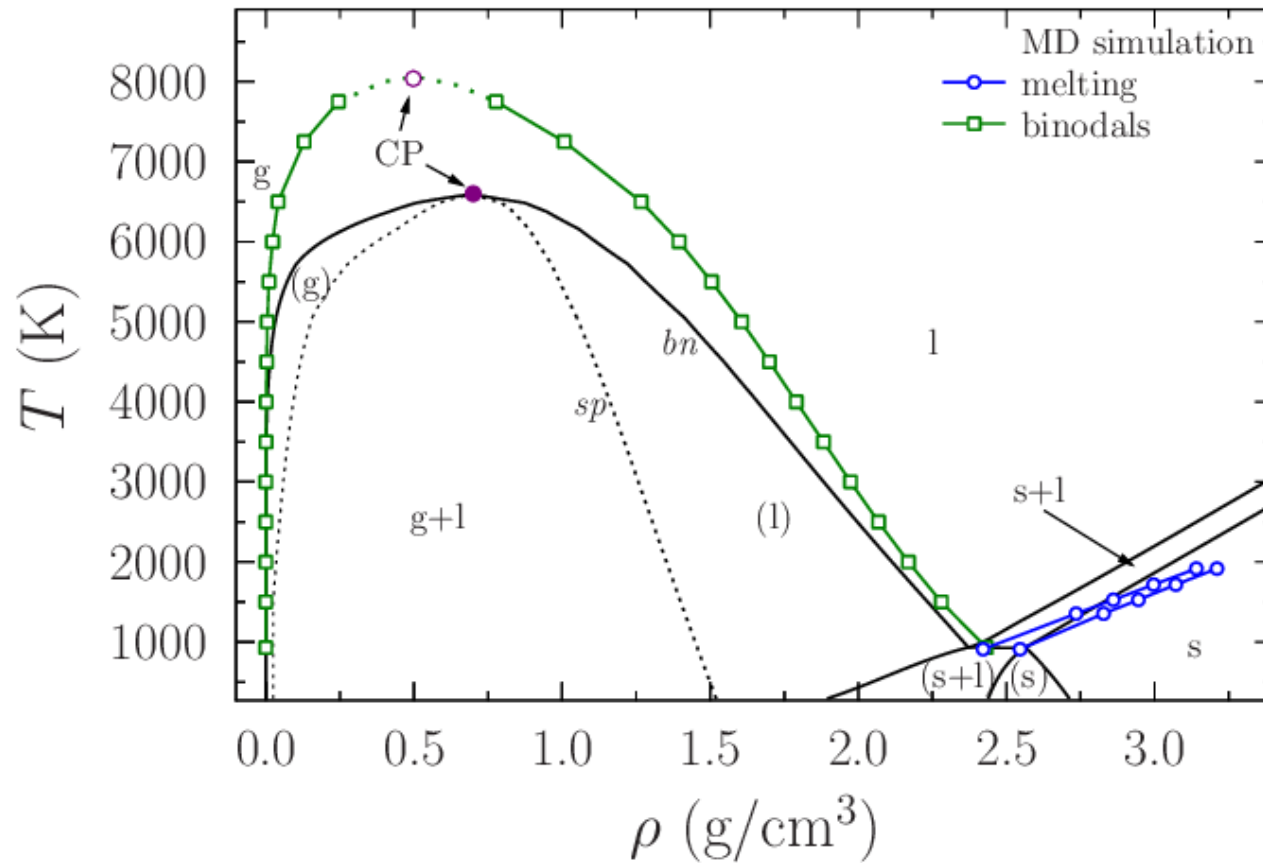
Lennard-Jones-like potential vs EOS

$$\phi(r) = \begin{cases} 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6], & r \leq r_c \\ 0, & r > r_c \end{cases}$$

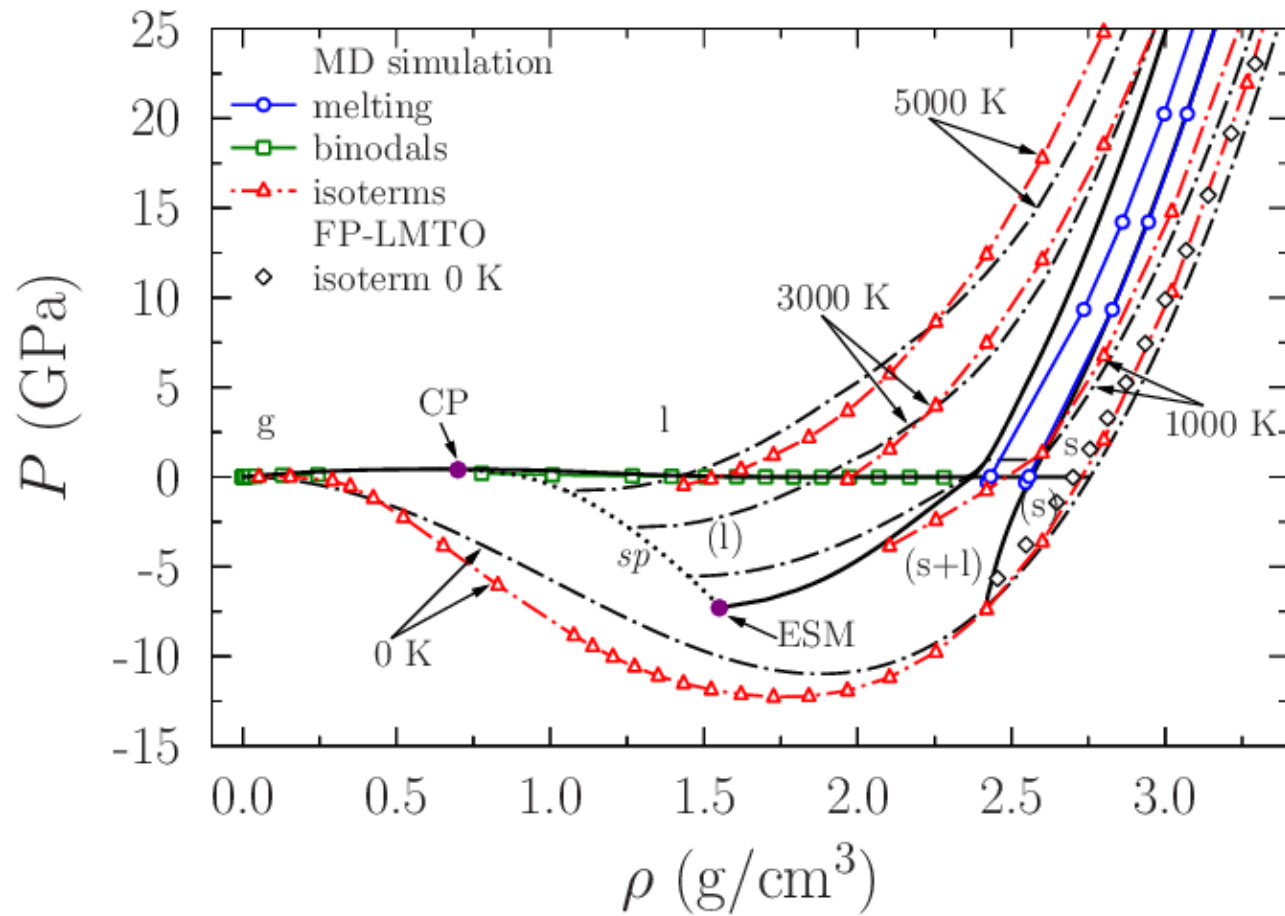


Bidakov *et al.* Fluid Phase Equilibria 263 (2008)

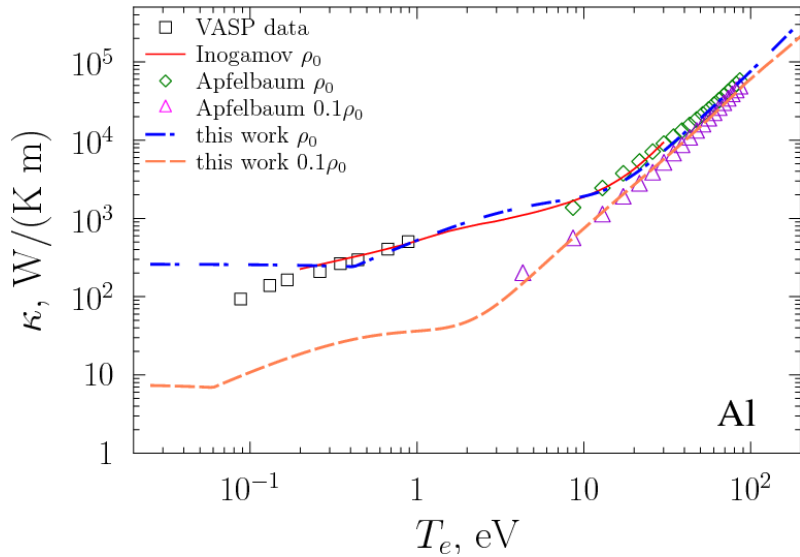
Eos vs phase diagramme obtained by MD/EAM



Eos vs phase diagramme obtained by MD/EAM



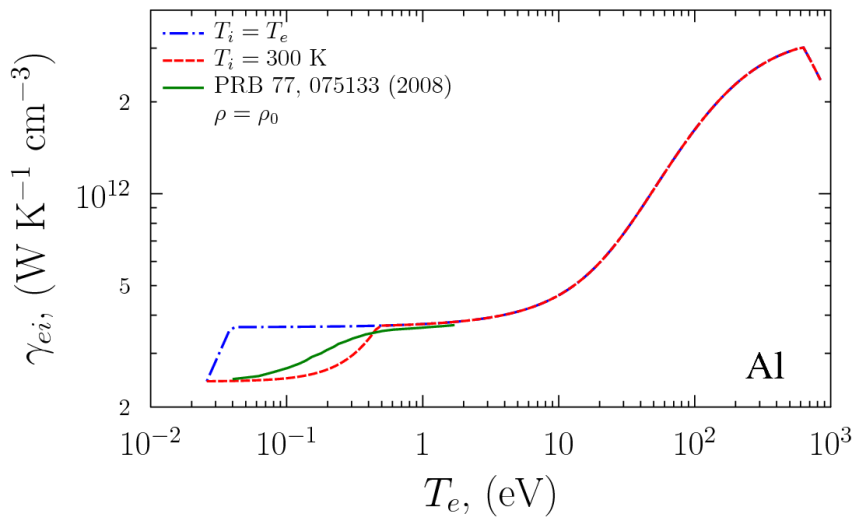
Thermal conductivity & electron-ion coupling



$$\kappa = \kappa_{\text{pl}} + (\kappa_{\text{met}} - \kappa_{\text{pl}})e^{-A_4' T_e/T_F}$$

$$\kappa_{\text{met}} = \frac{\pi^2 k_B^2 n_e}{3m_e \nu_{\text{eff},t}} T_e \quad T_e \ll T_F$$

$$\kappa_{\text{pl}} = \frac{16 \sqrt{2} k_B (k_B T_e)^{5/2}}{\pi^{3/2} Z e^4 \sqrt{m_e} \Lambda} \quad T_e \gg T_F$$



$$\gamma_{ei} = \frac{3k_B m_e}{m_i} n_e \nu_{\text{eff}}$$

Laser energy absorption (Helmholtz equation)

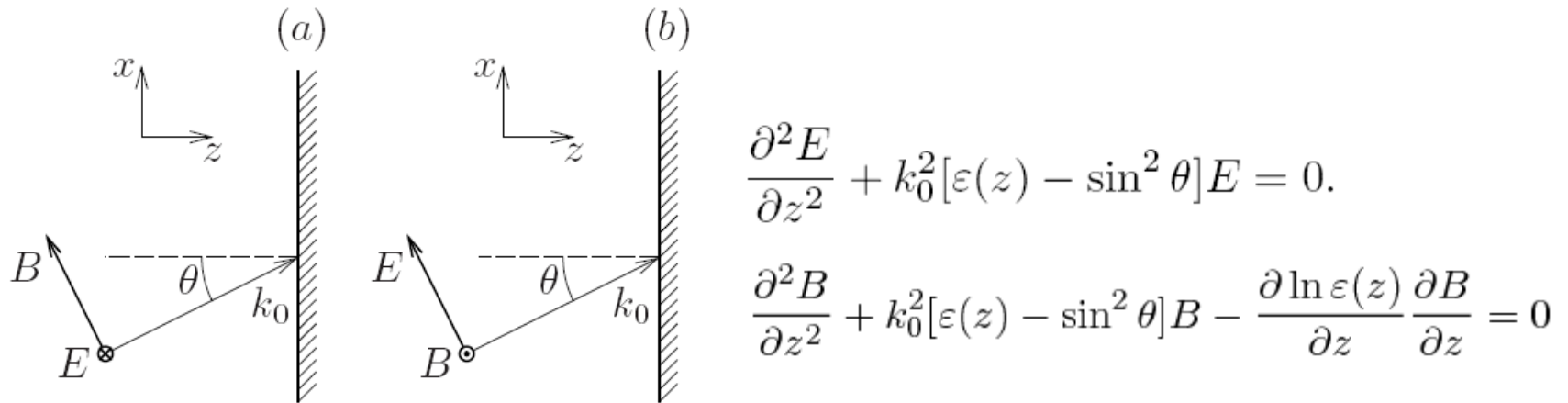
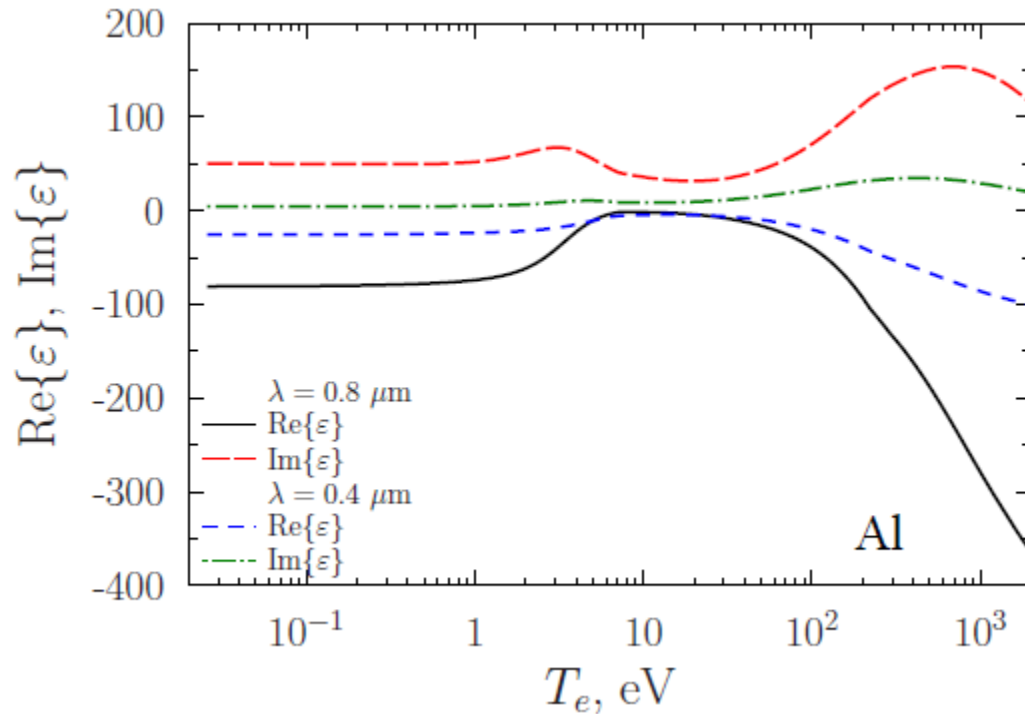


Figure 3. Polarization of laser light: (a)—s; (b)—p.

$$Q_L(t, z) = I(t) \frac{\omega_L}{c} \text{Im}\{\varepsilon(t, z)\} |E(t, z)/E_L(t)|^2$$

Dielectric function (for 400 and 800 nm)

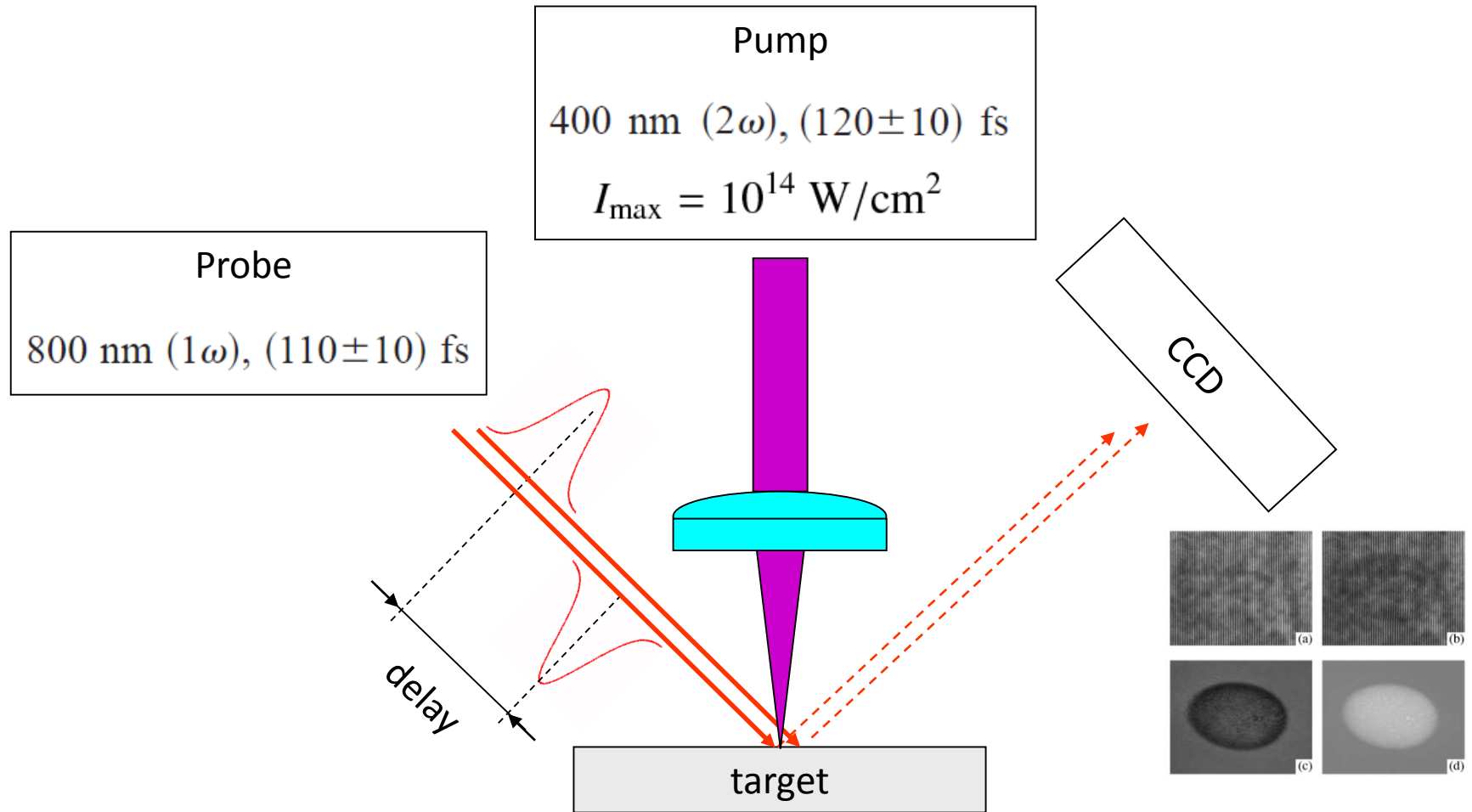


$$\varepsilon_{\text{met}}(\omega_L, \rho, T_i, T_e) = \varepsilon_{bb} + 1 - \frac{n_e}{n_{\text{cr}}(1 + i\nu_{\text{eff},p}/\omega_L)},$$

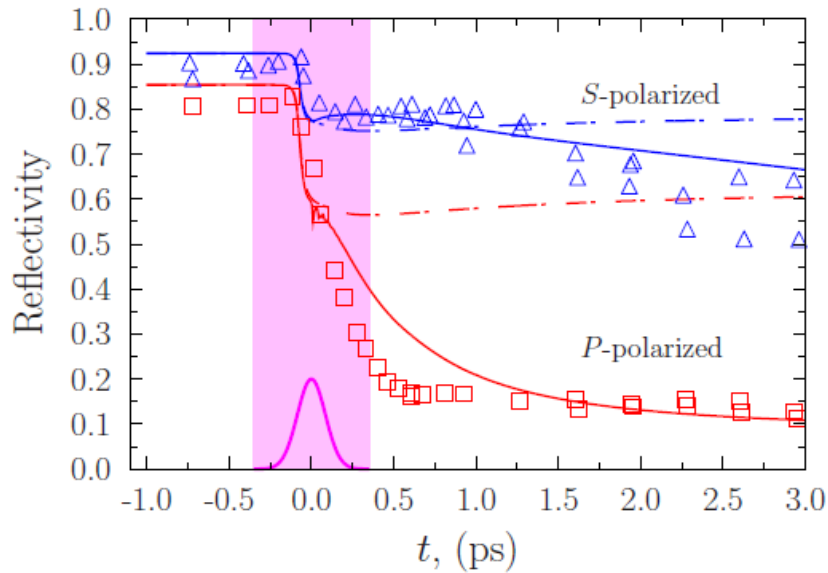
$$\varepsilon_{\text{pl}}(\omega_L, \rho, T_e) = 1 - \frac{n_e}{n_{\text{cr}}} \left[K_1(\xi) - i(\nu_{\text{pl}}/\omega_L)K_2(\xi) \right]$$

$$\varepsilon = \varepsilon_{\text{pl}} + (\varepsilon_{\text{met}} - \varepsilon_{\text{pl}})e^{-A_4^p T_e/T_F}$$

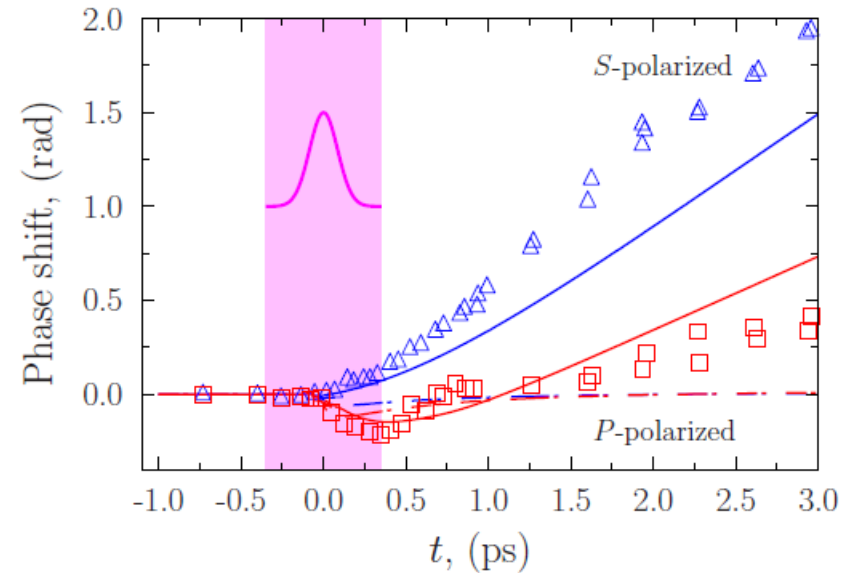
Pump-probe



Diagnostics using different laser polarizations (s- and p-)

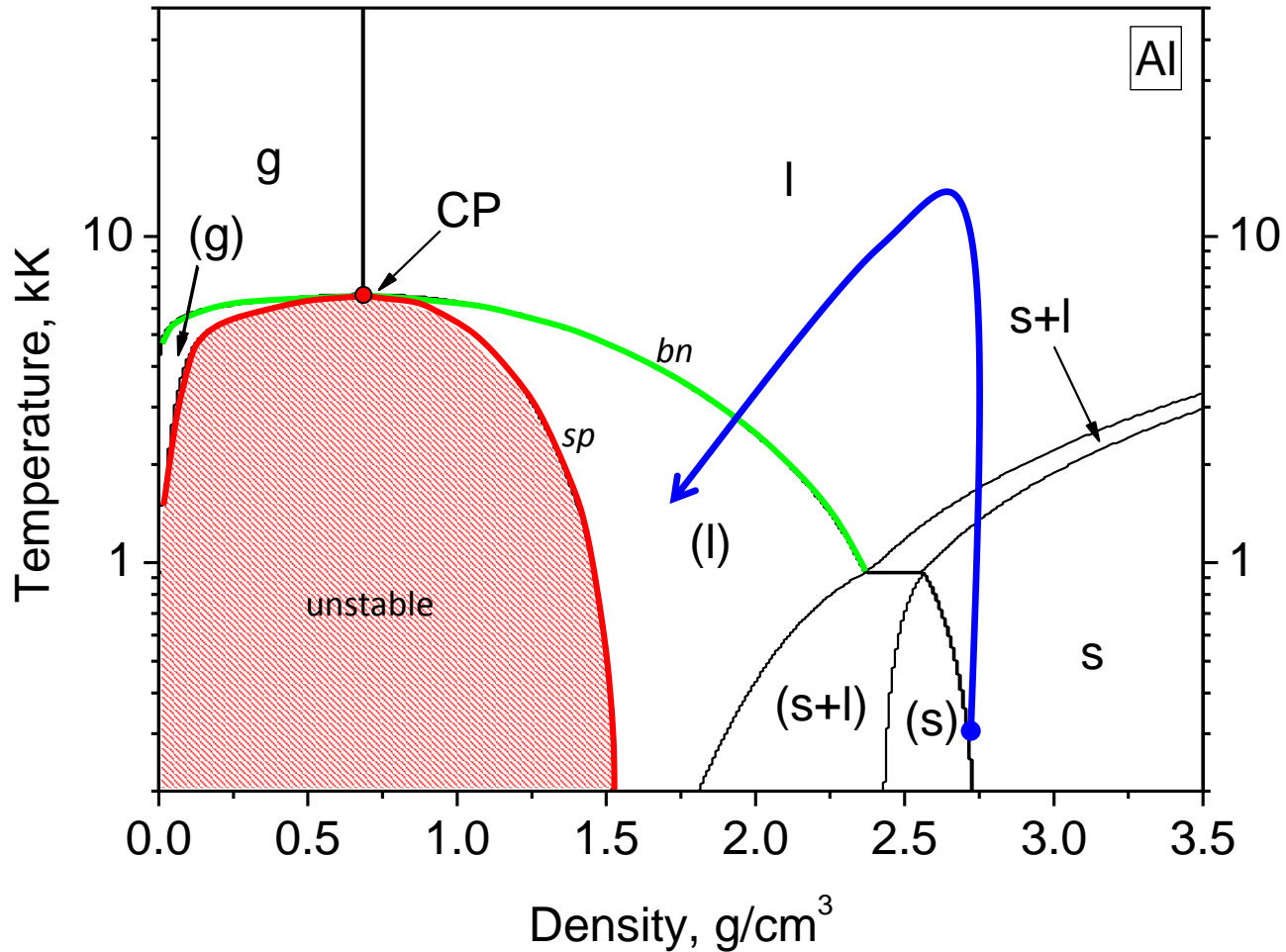


Reflectivity for s or p polarized probe lasers



Phase shift for s or p polarized probe lasers

Equation of state (EOS)



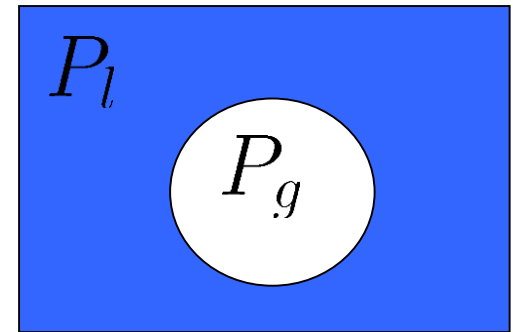
Nucleation

$$\tau_{\text{wait}} = (CN)^{-1} \exp(W/k_B T)$$

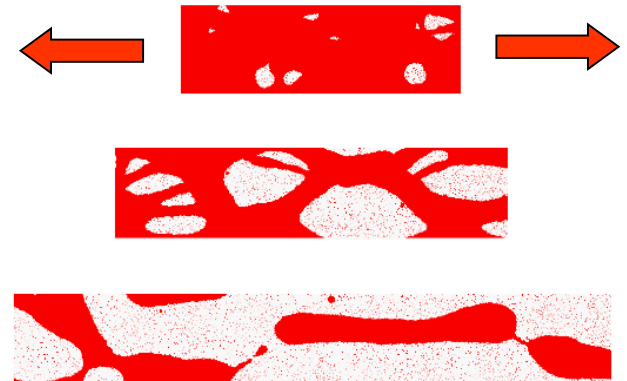
$$C \approx 10^{10} \text{ s}^{-1}$$

$$W = \frac{16\pi\sigma^3}{3(P_g - P_l)^2}$$

$$\tau_{\text{nucl}} = \tau_{\text{wait}} + \tau_{\text{grow}}$$

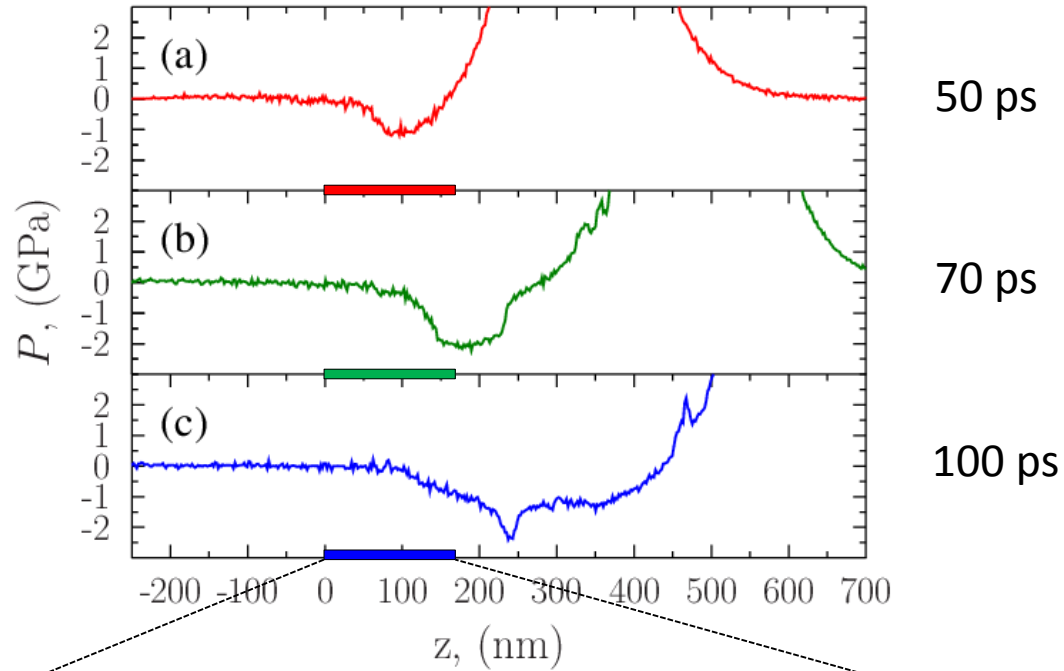


$$P_g > P_l + \frac{2\sigma}{R}$$

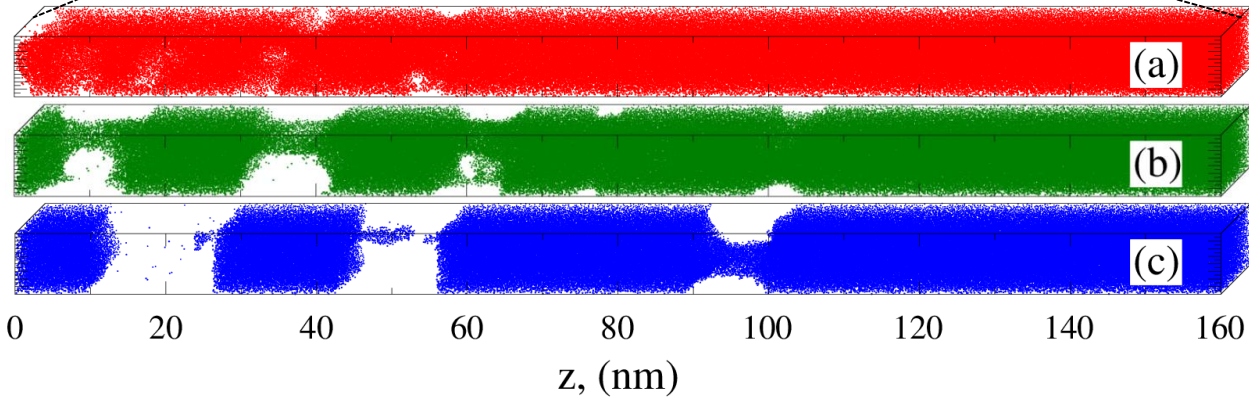


Pressure

Al, $F = 2.6 \text{ J/cm}^2$ (DM-TTM)



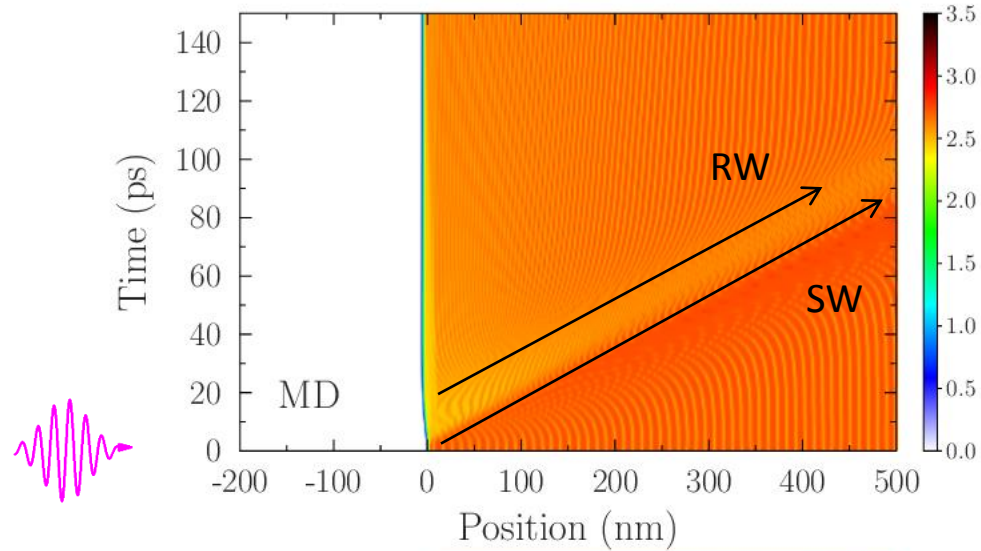
Laser



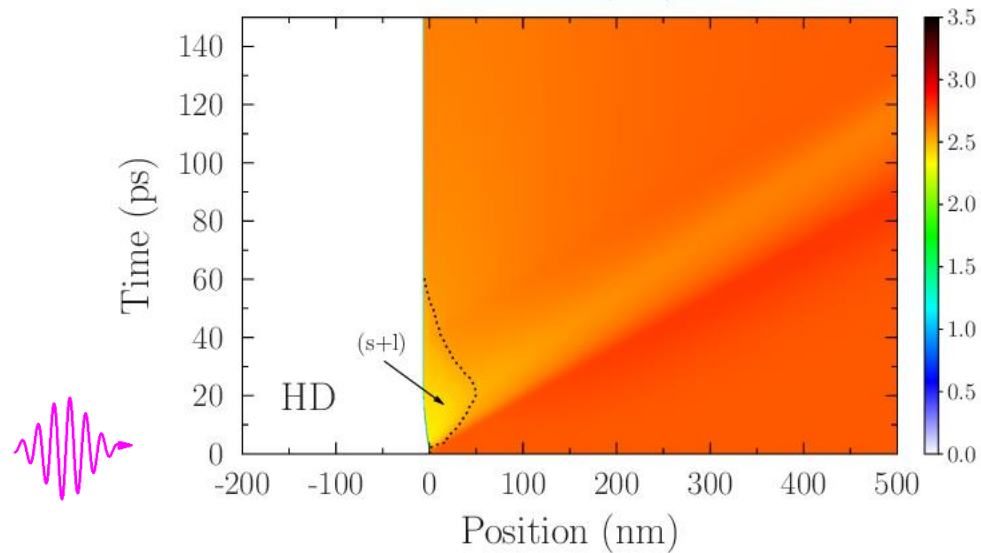
Density

$$\text{Al, } F = 0.2 \text{ J/cm}^2$$

TTM-MD



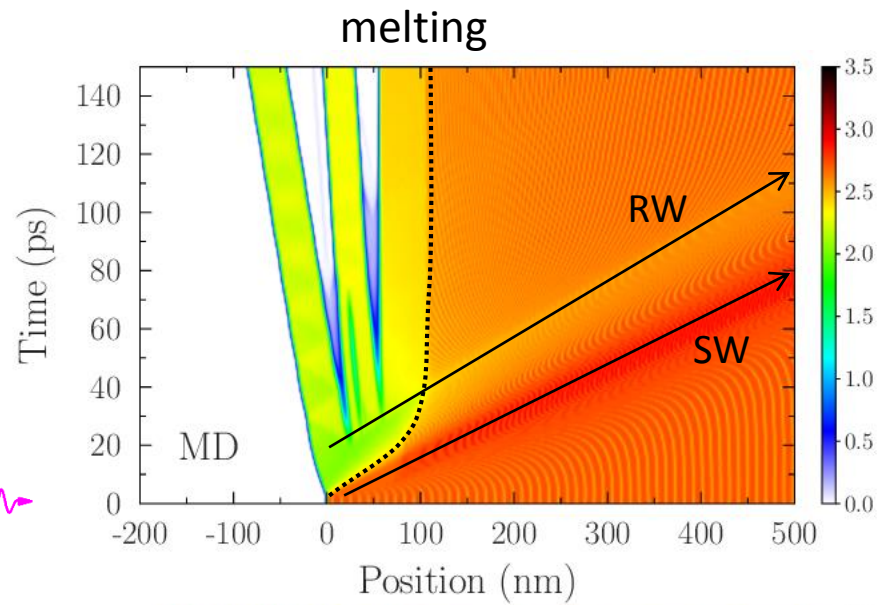
Hydrodynamics



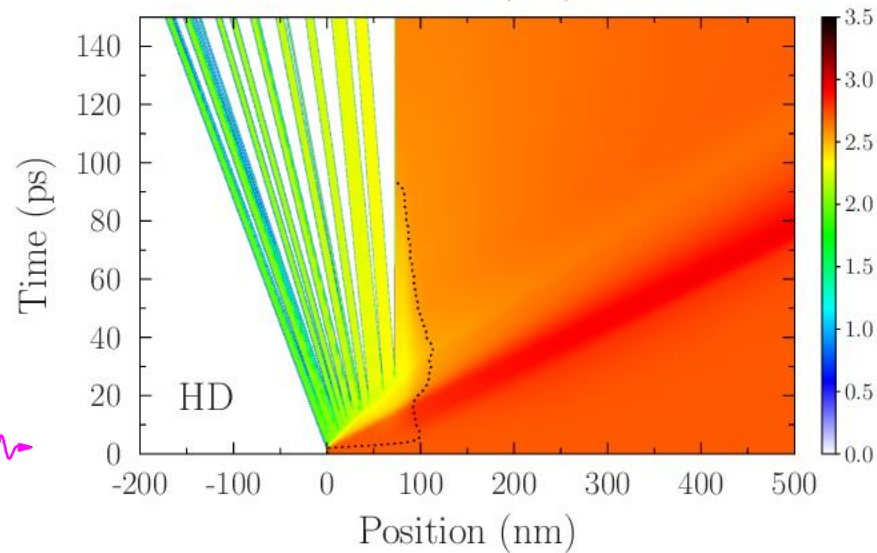
Density

$$Al, F = 0.5 \text{ J/cm}^2$$

TTM-MD



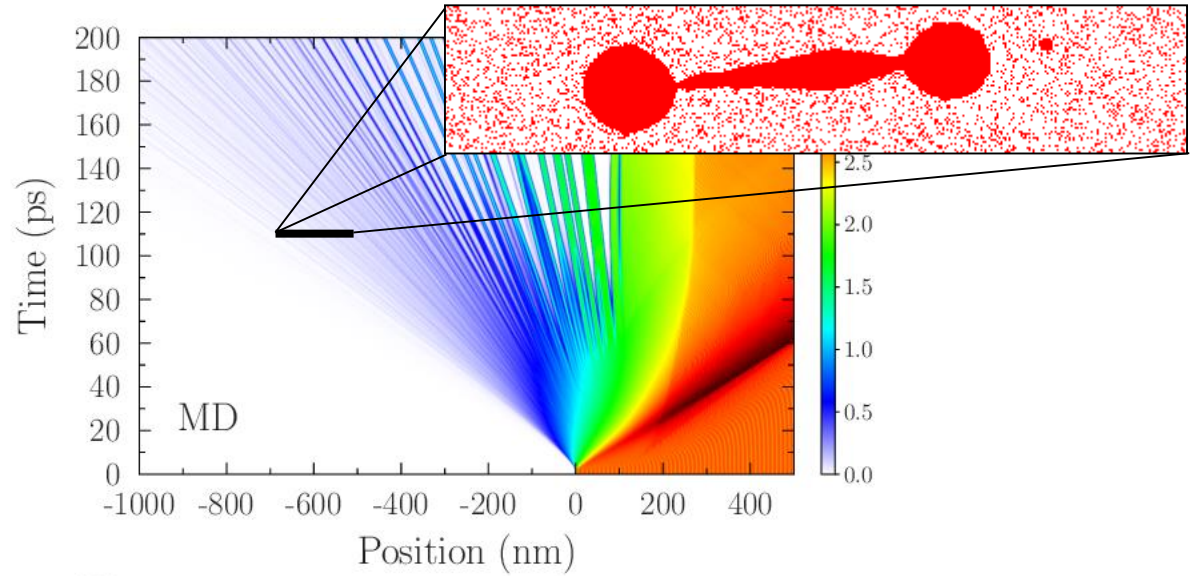
Hydrodynamics



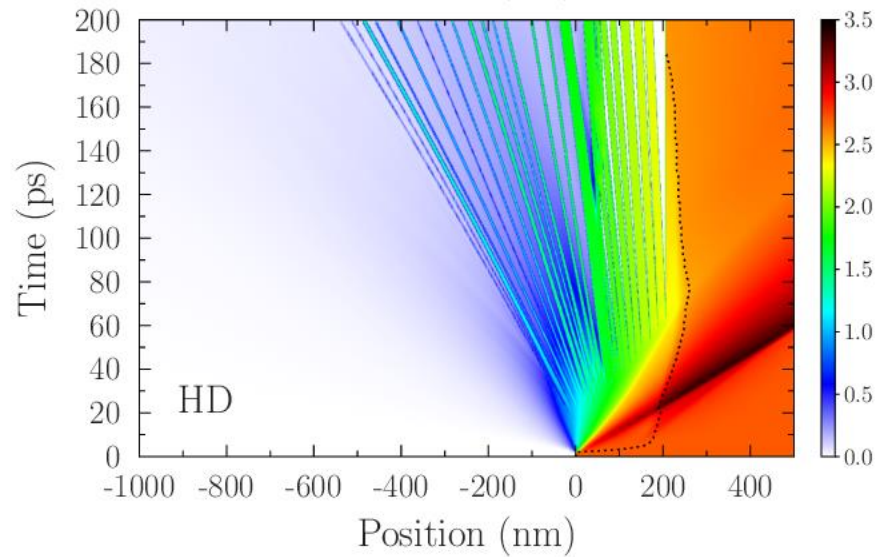
Density

$$\text{Al}, F = 2 \text{ J/cm}^2$$

TTM-MD



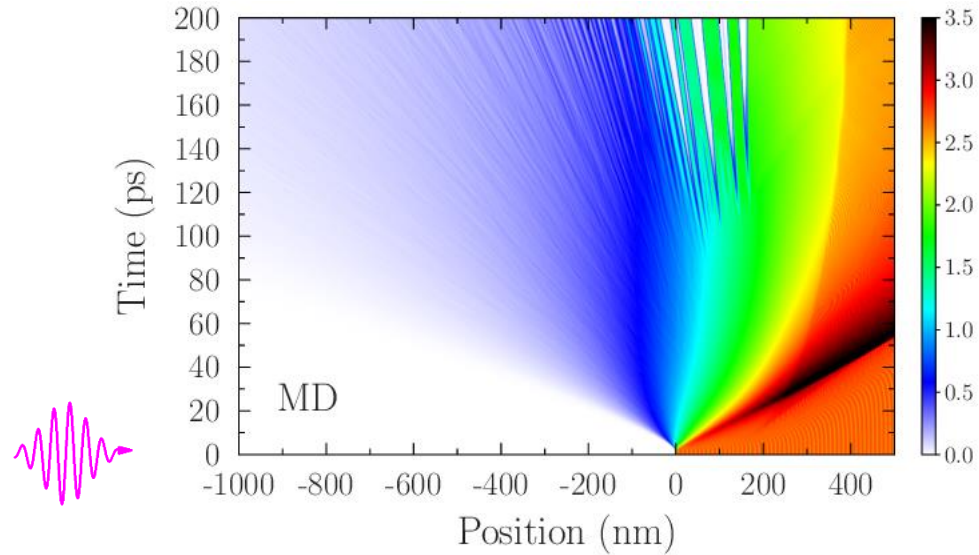
Hydrodynamics



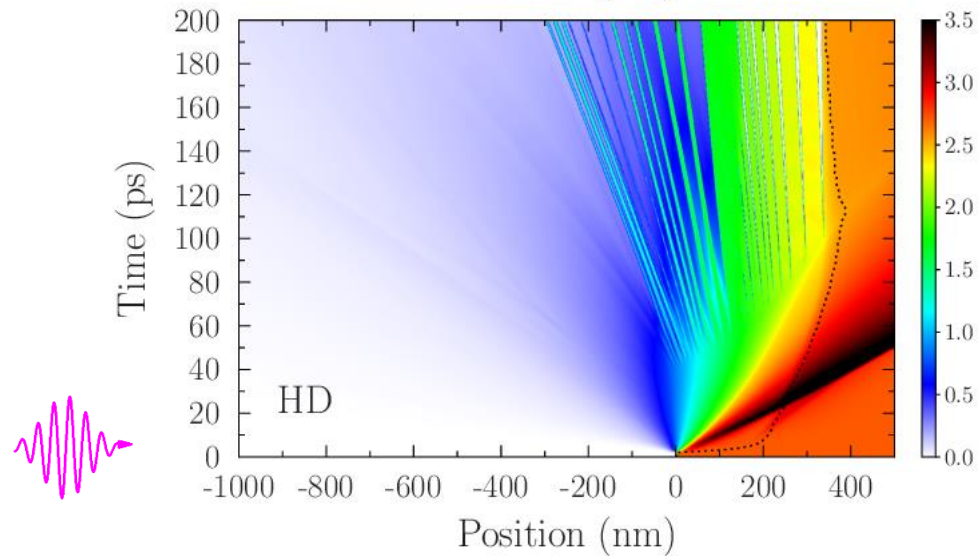
Density

$$\text{Al}, F = 4 \text{ J/cm}^2$$

TTM-MD



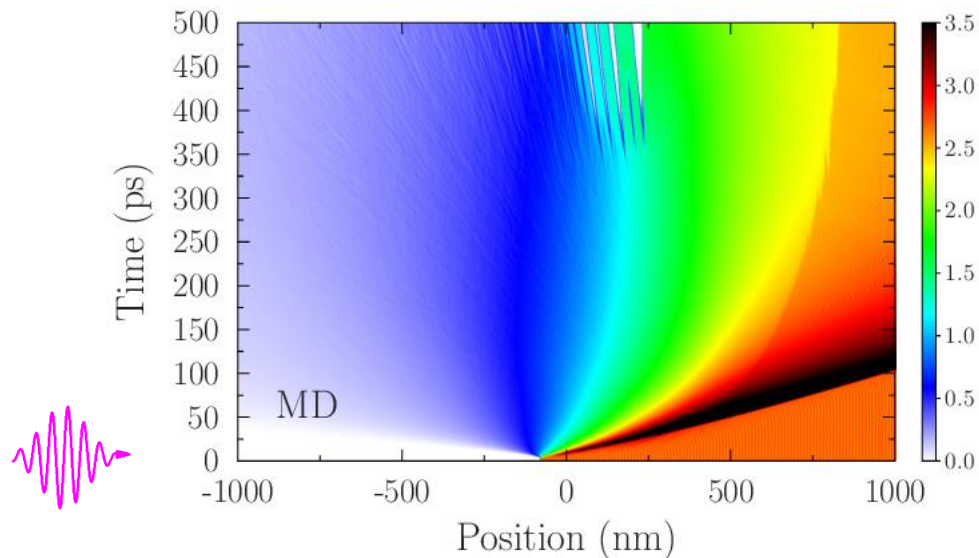
Hydrodynamics



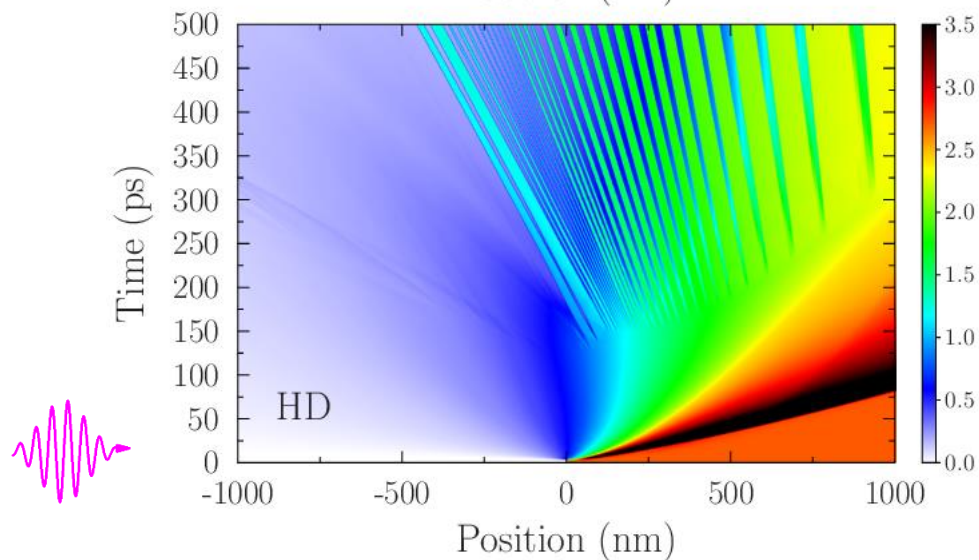
Density

$$\text{Al, } F = 20 \text{ J/cm}^2$$

TTM-MD

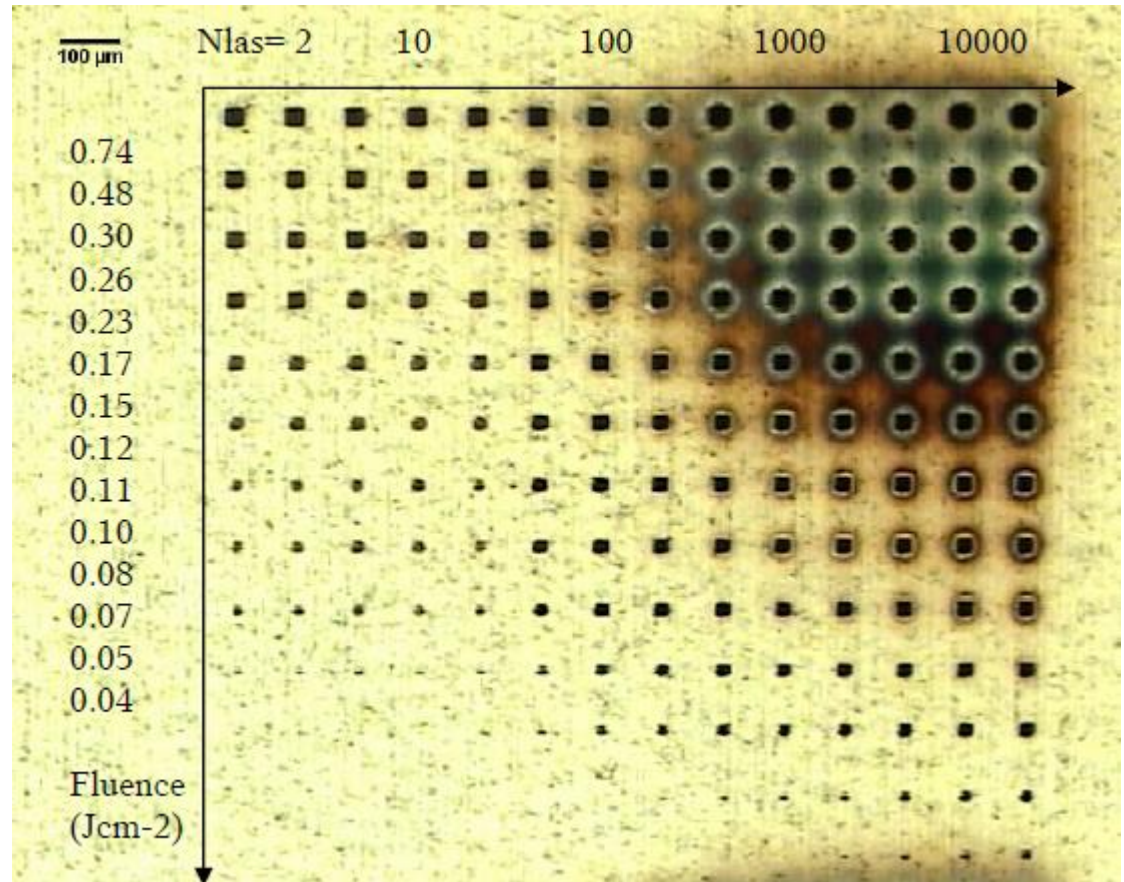
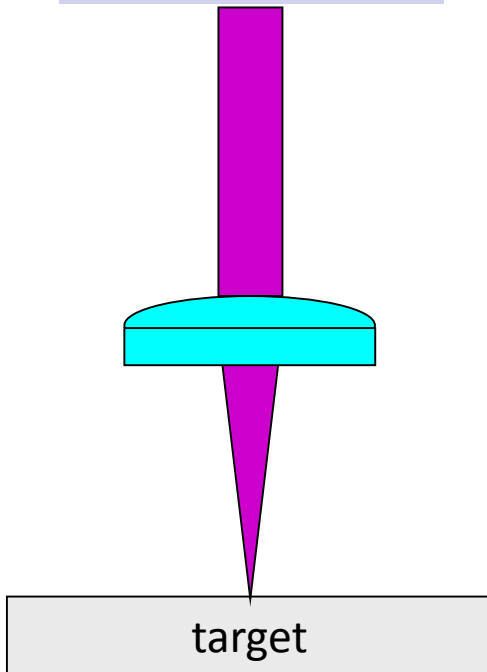


Hydrodynamics



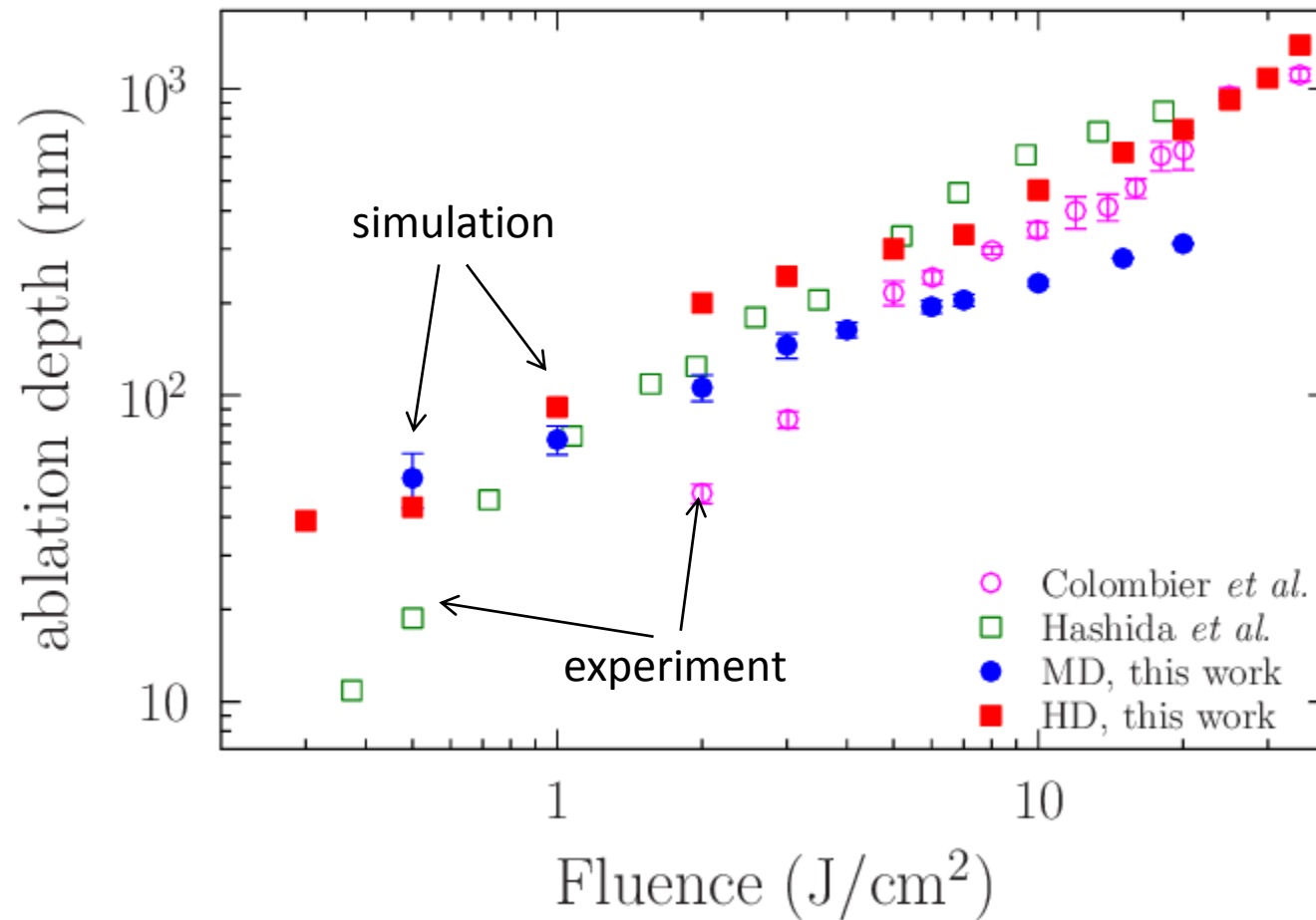
Experimental verification

$\lambda = 800 \text{ nm}$
 $\tau = 100 \text{ fs}$
 $F = 0.1 - 10 \text{ J/cm}^2$



Ablated depth vs laser fluence

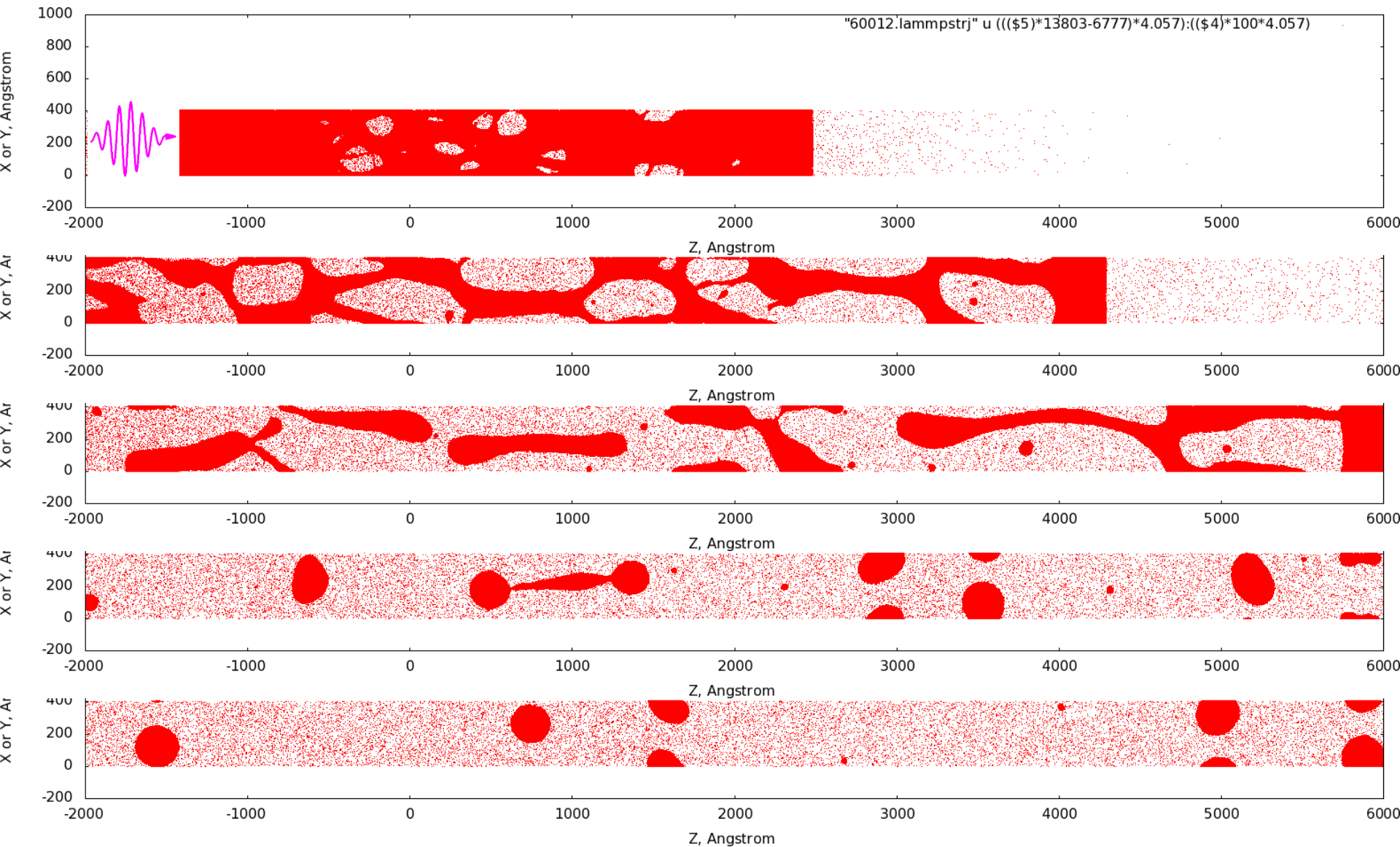
100 fs Al



MD-TTM vs HD-TTM

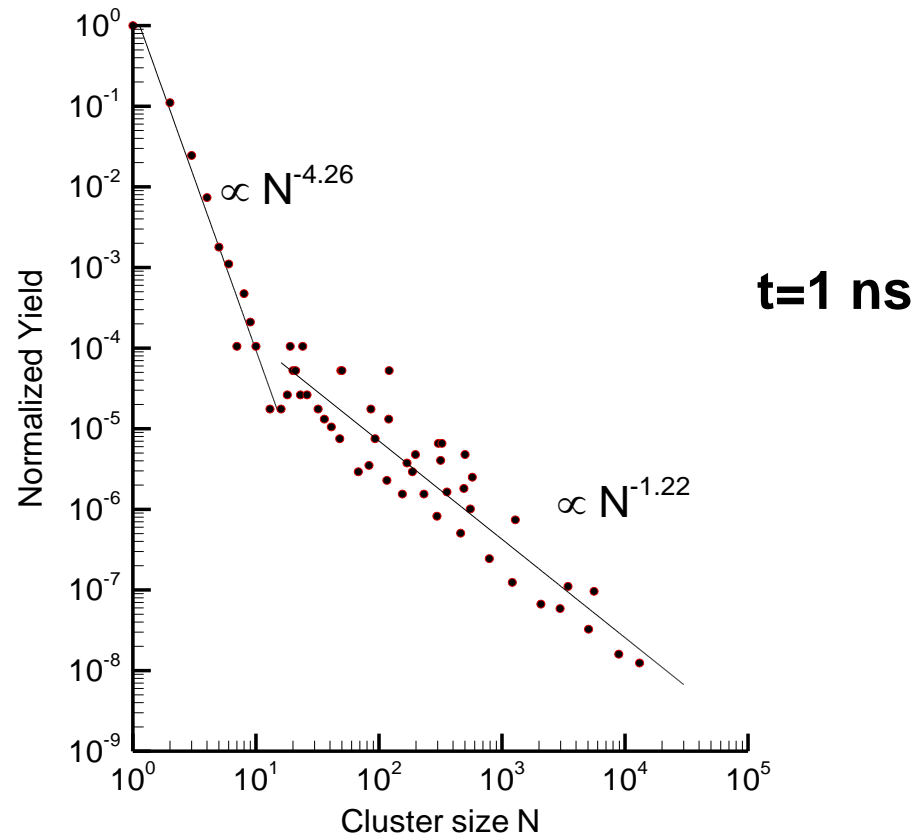
	DM-TTM	HD-TTM
Time step	~1 fs	~1 fs
Mesh	~1 nm	~1 nm
Calculation time	≈8 h, 360 cores	≈1 min, 1 core
Nucleation	Depends on potential	Nucleation model
Melting	Depends on potential	(EOS)
Condensation	Depends on potential	Condensation?
Phase state	Given by potential	EOS
Ionization	Not easy to include (T,Z)	Models

Ablation & nanoparticles (10M atoms, $F=1 \text{ J/cm}^2$, Al)



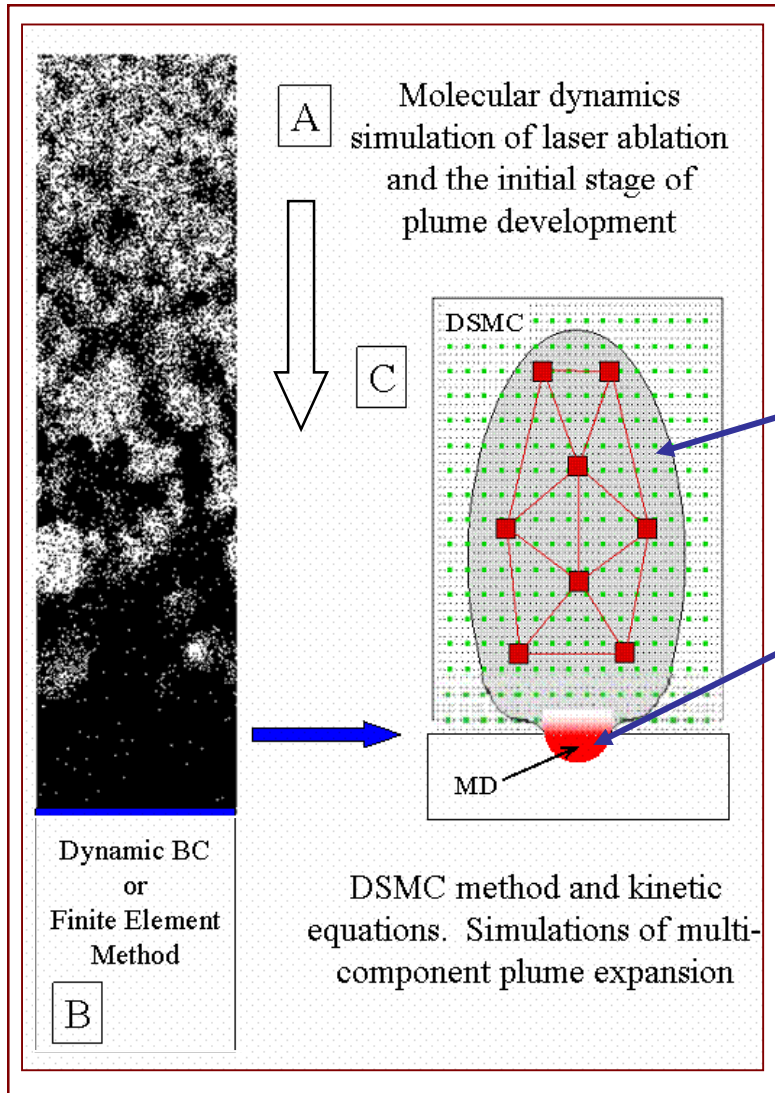
MD Simulations

=>nanoparticle size distributions



$\tau = 15 \text{ ps}$, $F \sim 2 \text{ Fth}$, $40 \times 10 \text{ nm}$, $t = 1 \text{ ns}$

Combined MD-DSMC



Combinaton

– Direct Simulation Monte Carlo

– Molecular Dynamics

Detailed information

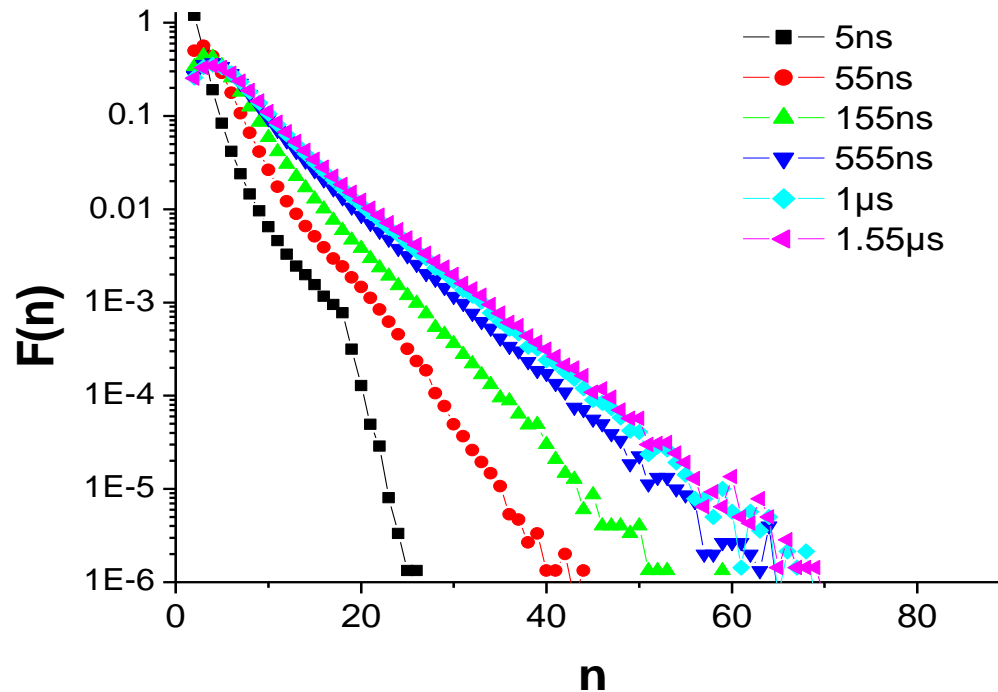
Continuous plume

Size distribution of aggregates

K. Gouriet, thèse (2008)

Growth of aggregates in an ablation plume

Laser ablation of a carbon target under vacuum (12 ps laser)

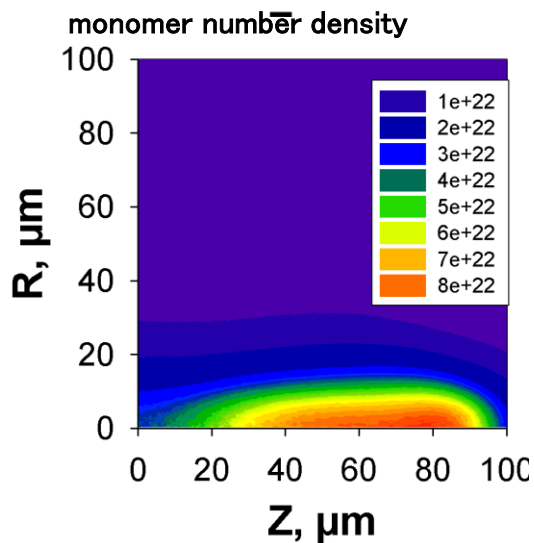
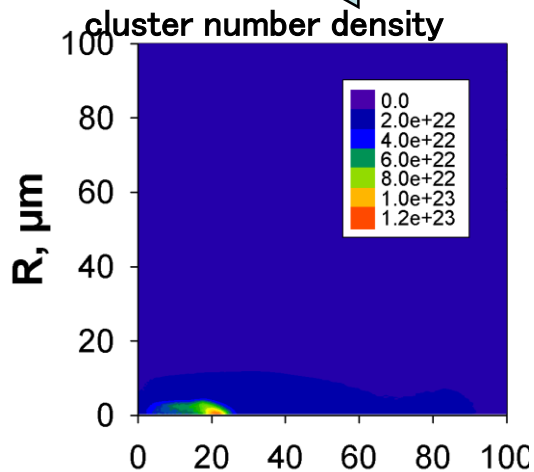


- growth $\Rightarrow 1.5 \mu\text{s}$,
- then, plume expansion, fewer collisions

MD-DSMC

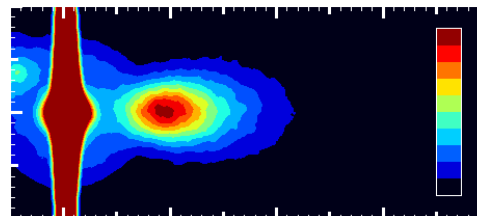


$$F_{las} = 4 \text{ Jcm}^{-2}$$

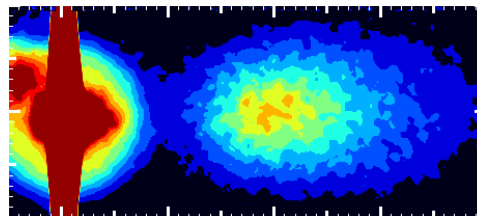


Numerical results

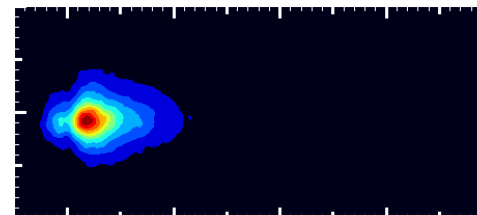
$t = 50 \text{ ns}, 15 \text{ ps}, F = 61 \text{ J/m}^2, R = 10 \text{ μm}$



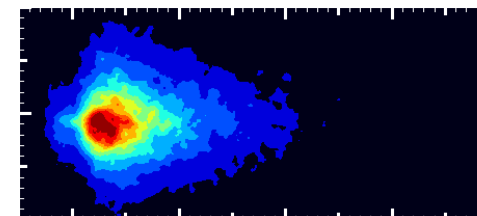
200 ns



400 ns



5 μs



10 μs

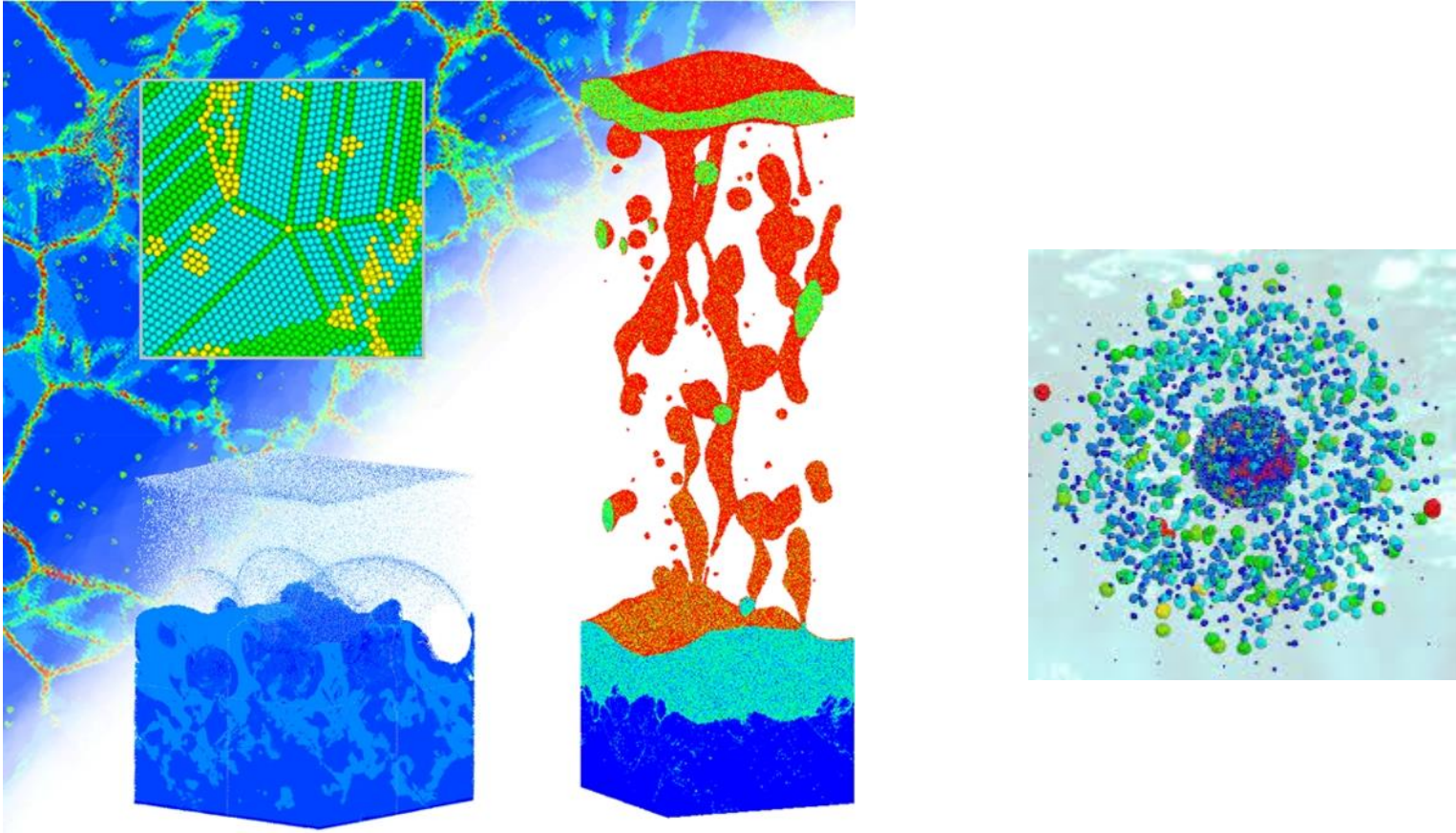
0 1 2 3 4 (mm)

Experimental results (J. Hermann, S. Noël)

100 fs $F = 4 \text{ J/cm}^2$

Tiny zaps, big results

There is big science in the tiny realm of nanotechnology...



Courtesy Leonid Zhigilei, VSU, USA

<https://sciencenode.org/feature/tiny-zaps,-big-results.php>

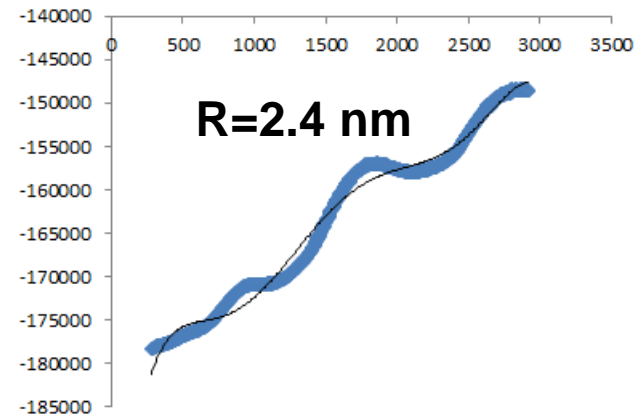
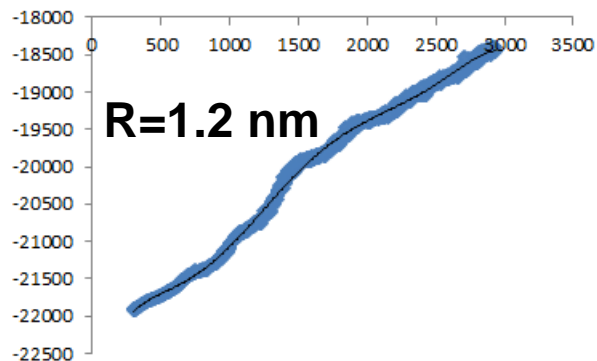
Ultra-short Laser interaction with a single Au NP in vacuum

MD simulations

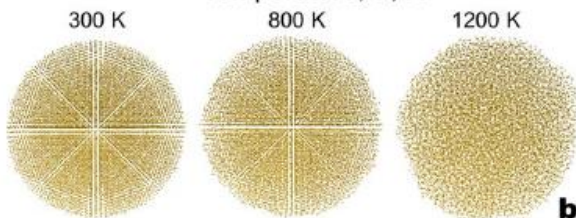
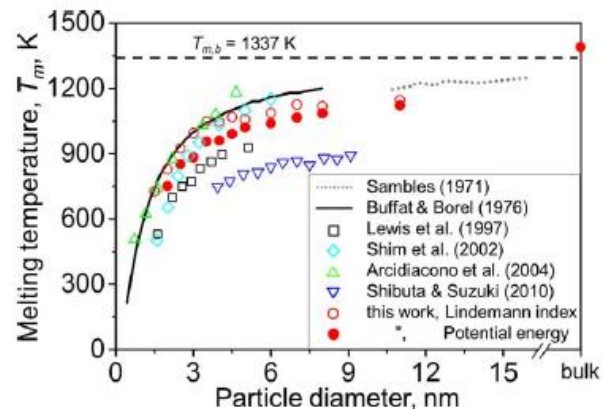
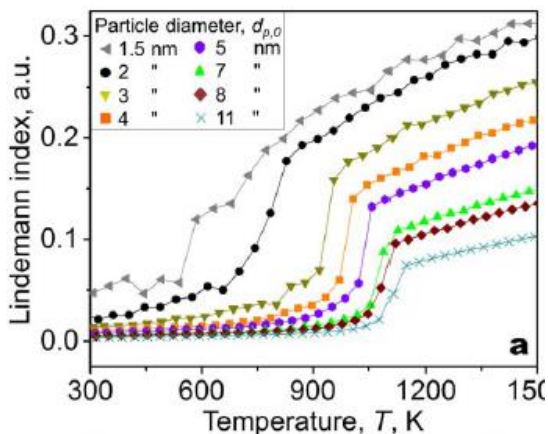
Au

R=1.2 nm and 2.4 nm

Time-evolution of potential energy, rapid heating



Melting and ... structural transformations



E. Goudeli et al.,
AIChE 2015

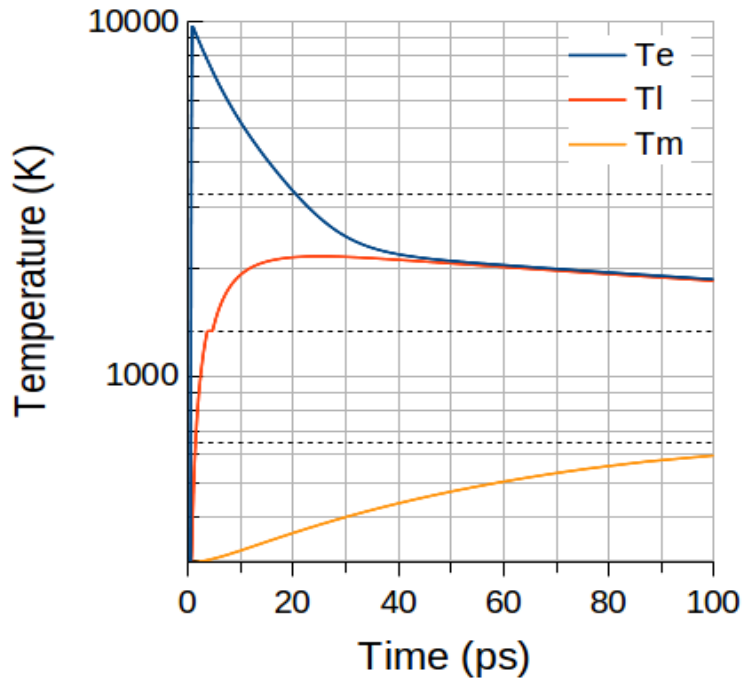
N_t



2e4

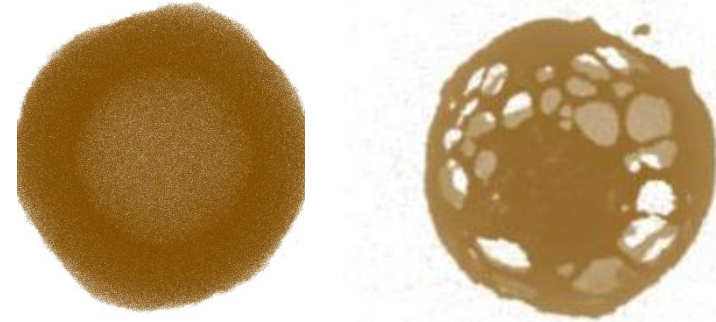
T.E. Itina at al.

Ultra-short Laser interaction with a single Au NP in liquid



MD simulations

Heating during e-ph coupling

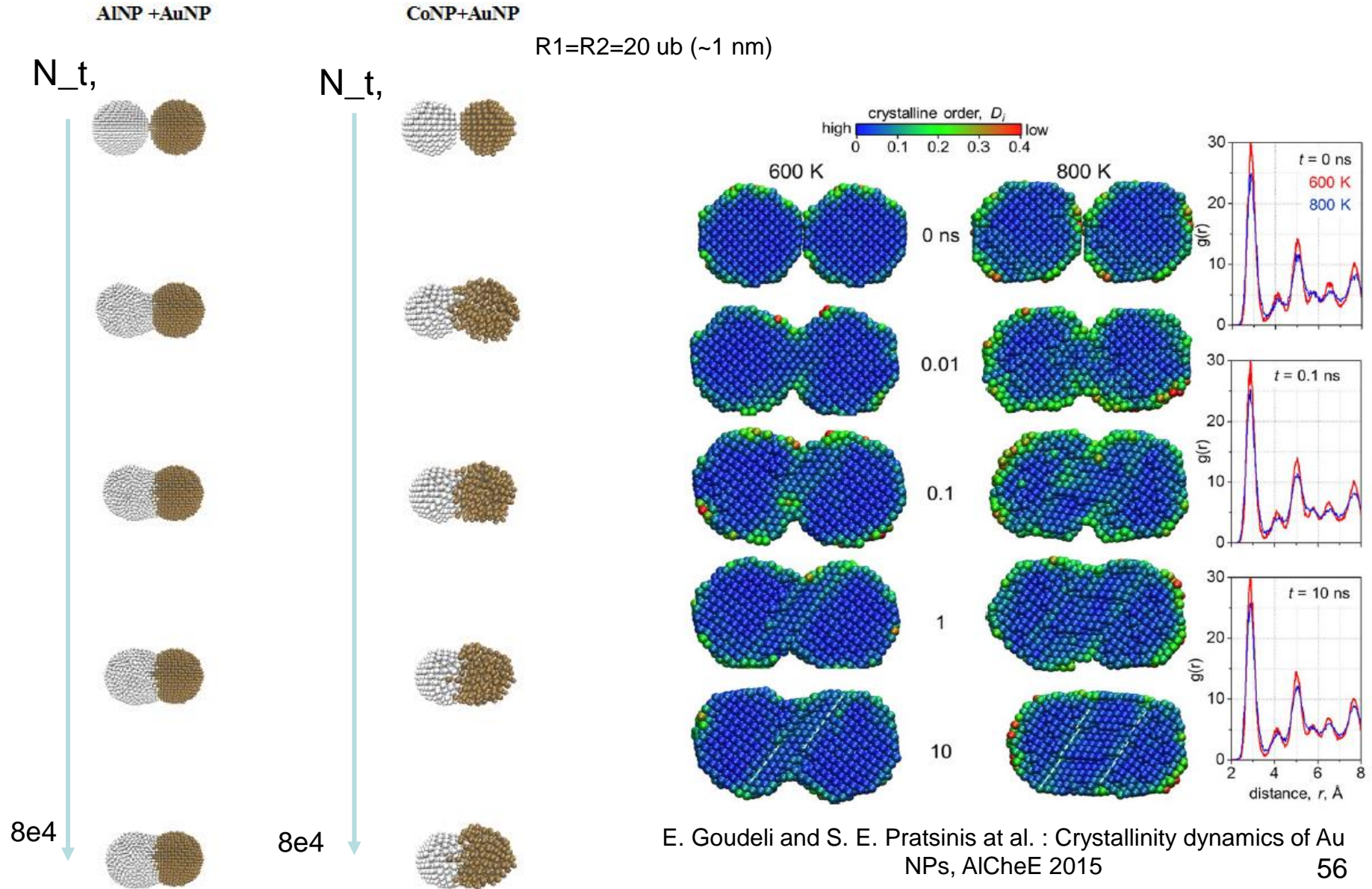


In liquids, surface is cooled down, so that NP faster cooling affects the final configuration

30 nm radius gold particle in water
absorbing laser pulse of **150 fs** at **400 nm**
with laser fluence of **12.3 mJ/cm²**
Gaussian time profile

Ultra-short Laser-induced NP sintering, Janus NPs

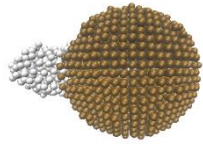
MD simulation results



E. Goudeli and S. E. Pratsinis et al. : Crystallinity dynamics of Au NPs, AIChE 2015

Ultra-short Laser-induced NP hybrid (core-shell) formation

FeNP 1700+AuNP 1700



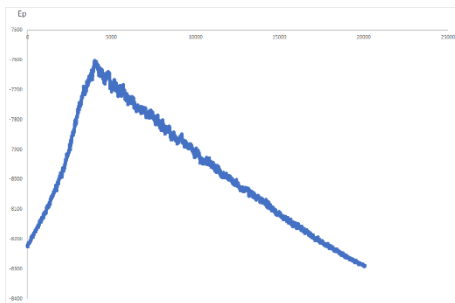
N_t



8e4

Different sizes
The same temperatures

Time-evolution of
potential energy

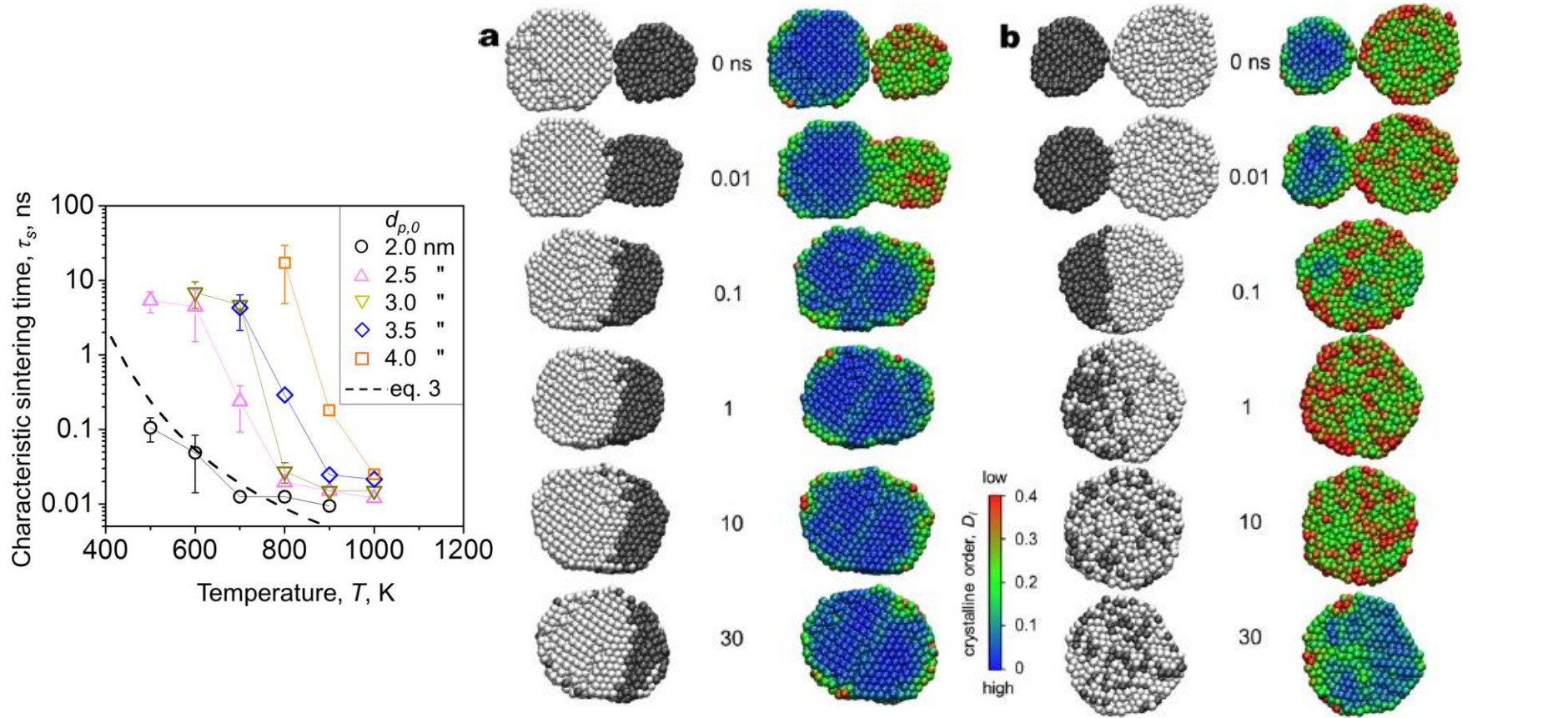


- Simulation starts from a Janus configuration
- Then both particles are heated to the same temperature
- Then, the system is cooled down back to room temperature

Core-shells can be formed when one particle is larger

Ultra-short Laser-induced NP sintering, Janus NPs

AuNP + AuNP, different sizes



Snapshots of cross-sections of two Au nanoparticles with $d_{p,0}=3$ (gray) and 4 nm (white) undergoing sintering at $T = 800$ K at $t = 0, 0.01, 0.1, 1, 10,$ and 30 ns.

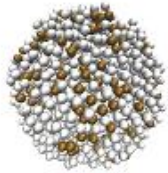
Ultra-fast heating and cooling of alloy NP

AlAuNP, 20% T=1200K

AlAuNP, 80% T=1200K

0.1 nm

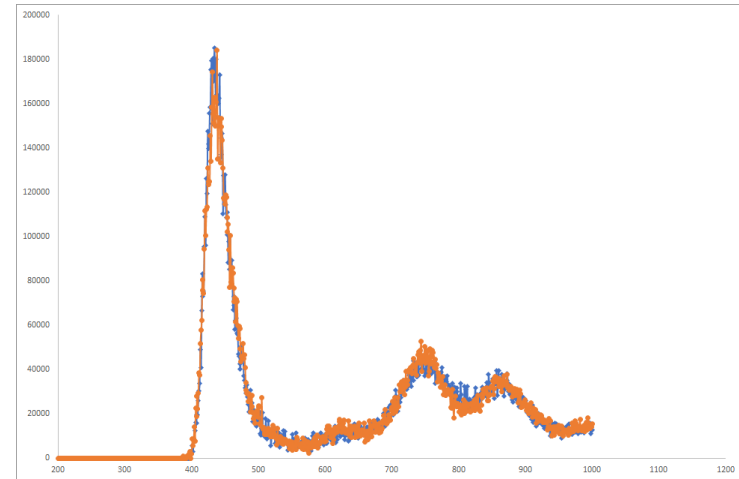
N_t



8e4

Different proportions of Au

Correlation function $g(r)$



When the percentage of Au is smaller, Au atoms tend to aggregate at the surface during NP cooling

When the percentage of Au is larger, the nanoparticles suffers less thermal expansion and is more stable



Thank you for your attention!

tatiana.itina@univ-st-etienne.fr