4th EMMI workshop on Plasma Physics with Intense Heavy Ion and Laser Beams
GSI, Darmstadt, May 2-4, 2011

From Warm Dense Matter to Defects Evolution Under Irradiation

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1. **Electron-temperature dependent interionic potential for Au**

2. **Picosecond laser ablation of Au**

3. **Radiation damage in Mo**

Electron-temperature dependent interionic potential for Au

2T Atomistic Model of Irradiation

- MD for ions + thermostat due to electrons

$$m\frac{d\vec{v}_i}{dt} = \vec{F}_i - \beta\vec{v}_i + A\vec{\xi}(t)$$

- Interionic potential: electron temperature dependent (ETD)

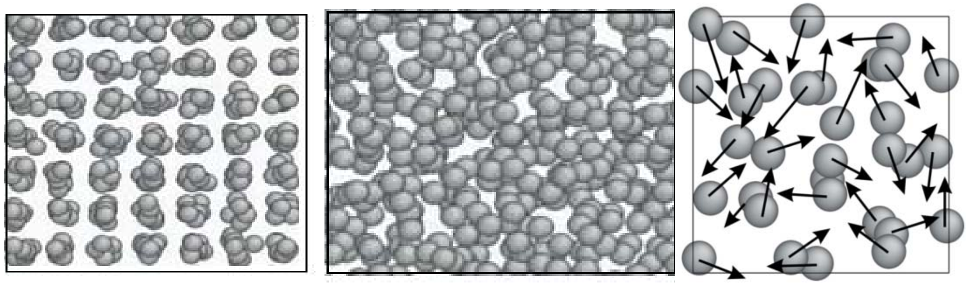
- Thermal conductivity equation for electronic subsystem:

$$C_e\frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - G_p(T_e - T_a)$$

Development of EAM potential: force matching to *ab initio* data

Configuration set
(+ per-atom forces, energies, stresses)

VASP

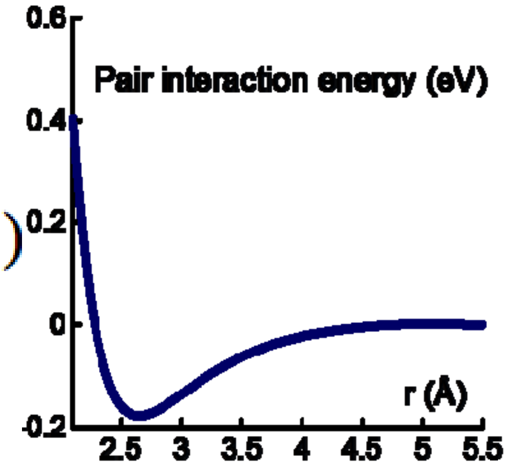


EAM potential

PotFit

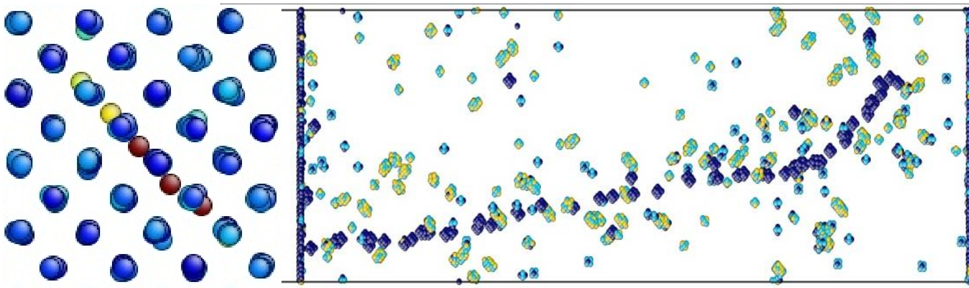
$$U = \sum_{i,j<i} \phi_{ij}(r_{ij}) + \sum_{i} F(\rho_i)$$

$$\rho_i = \sum_{j \neq i} \rho(r_{ij})$$

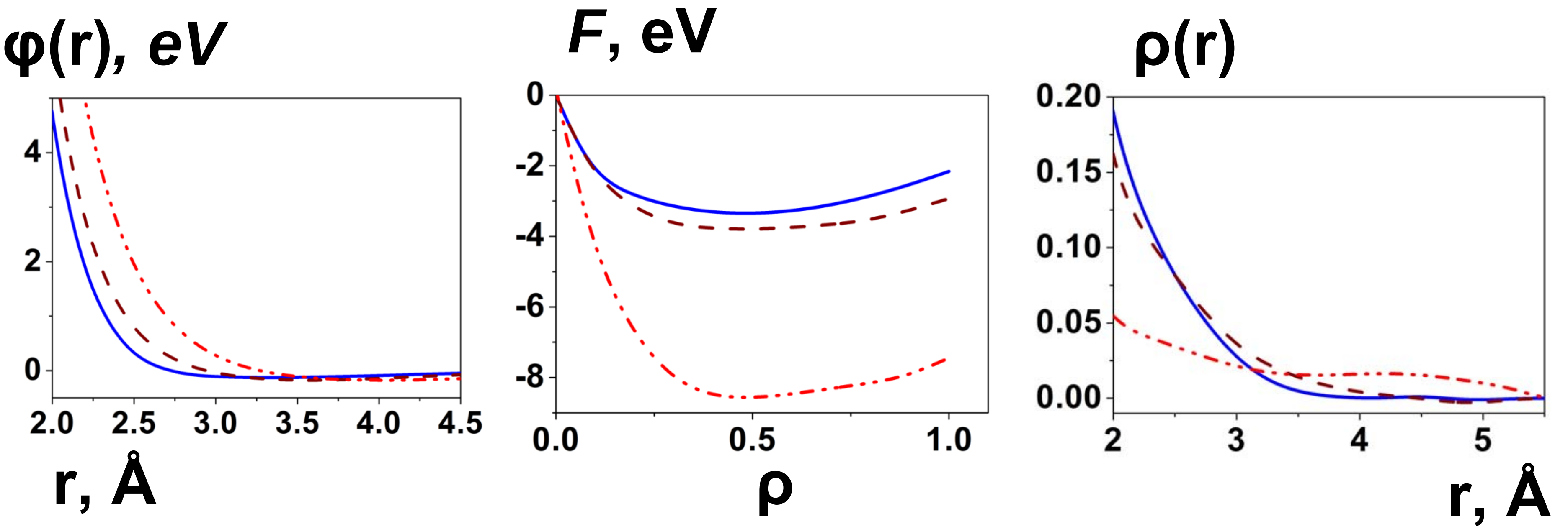


Static and kinetic characteristics

VASP
LAMMPS

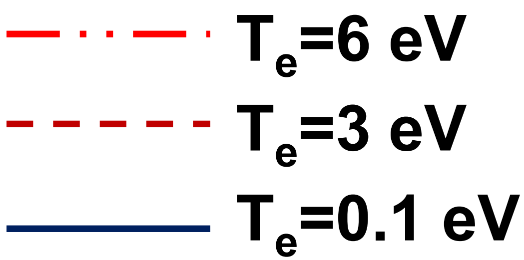


ETD-potential for Au

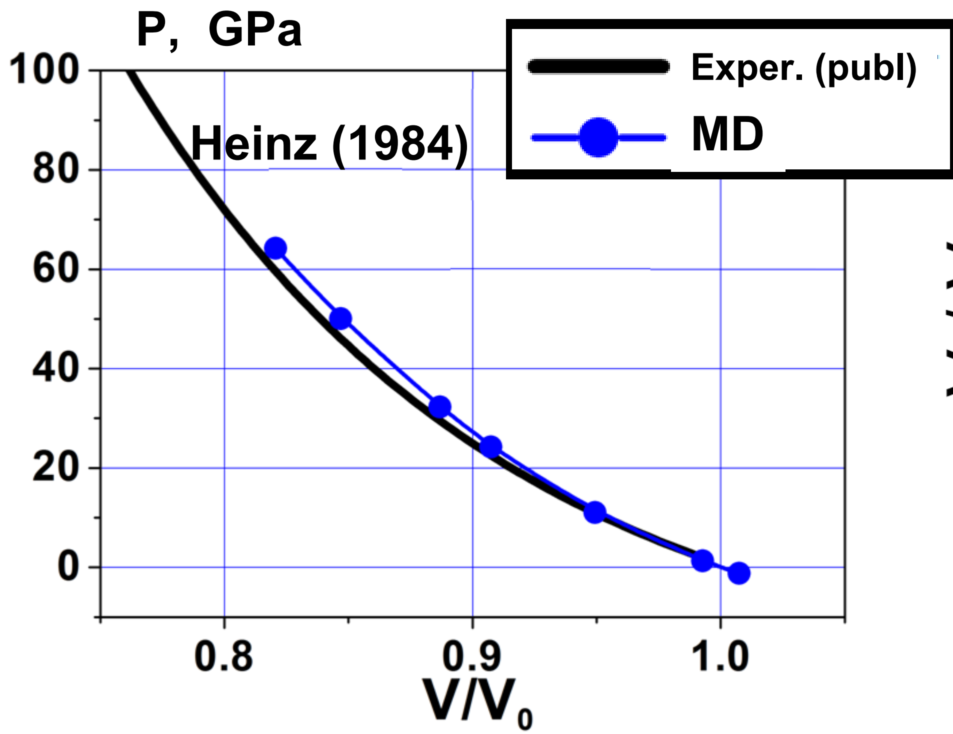


$$U = \sum_{i,\, j<i} \phi_{ij}(r_{ij}) + \sum_{i} F(\rho_i),$$

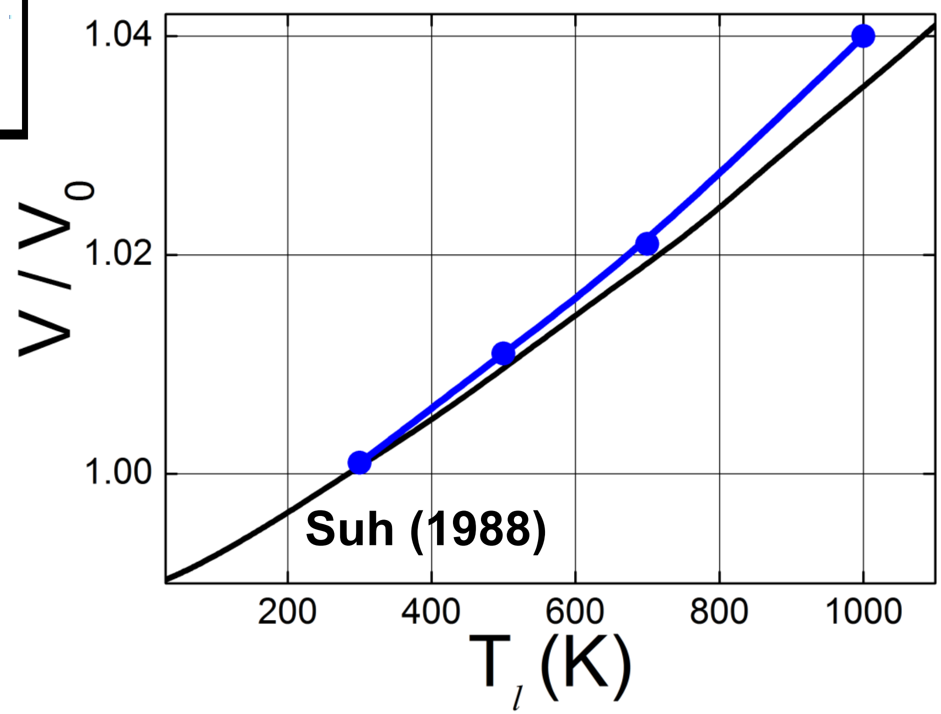
$$\rho_i = \sum_{j \neq i} \rho(r_{ij}) \qquad \text{(EAM)}$$



Verification of ETD-potential at T_e = 0.1 eV



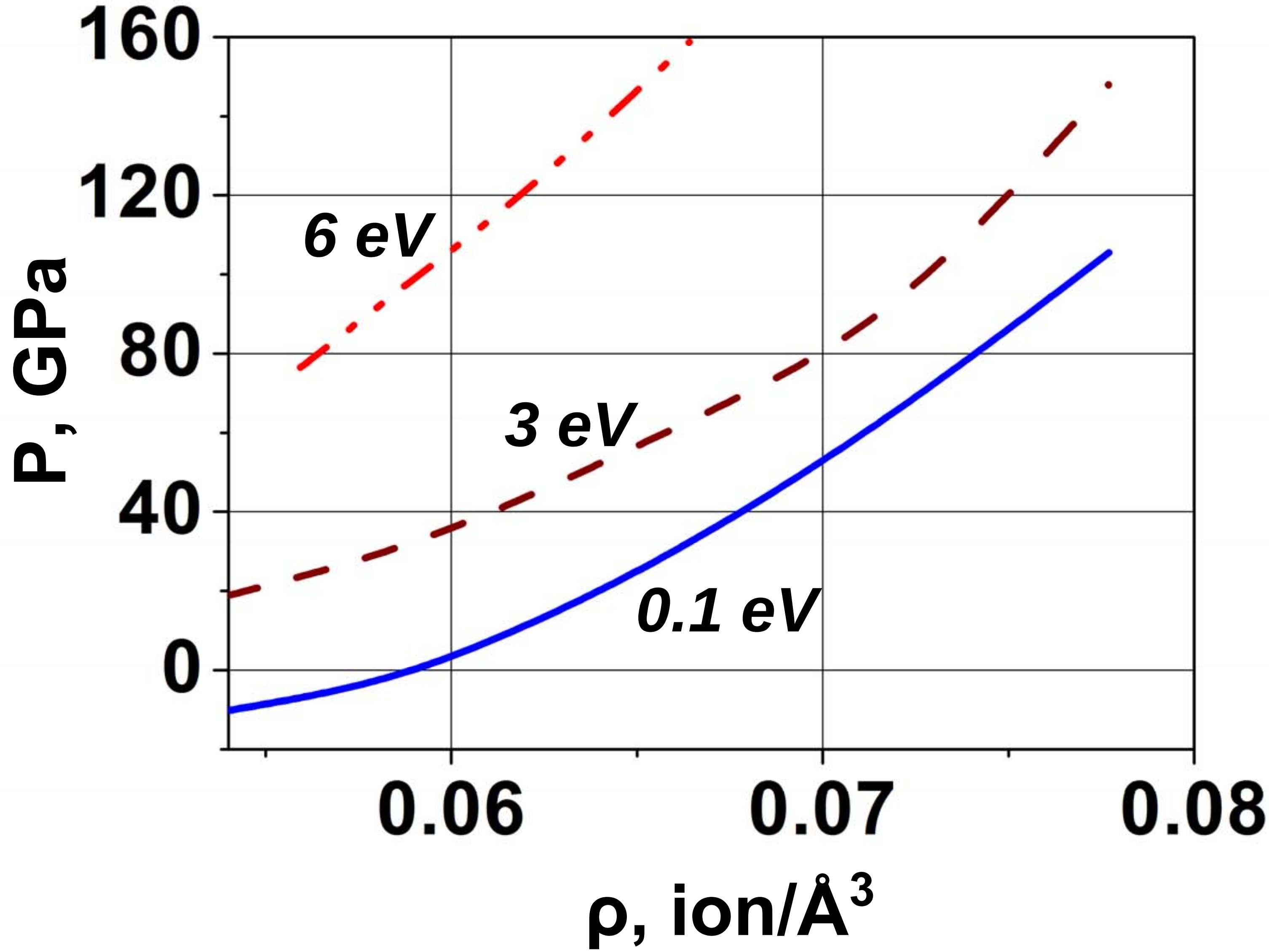
Cold curve Au



Thermal expansion Au

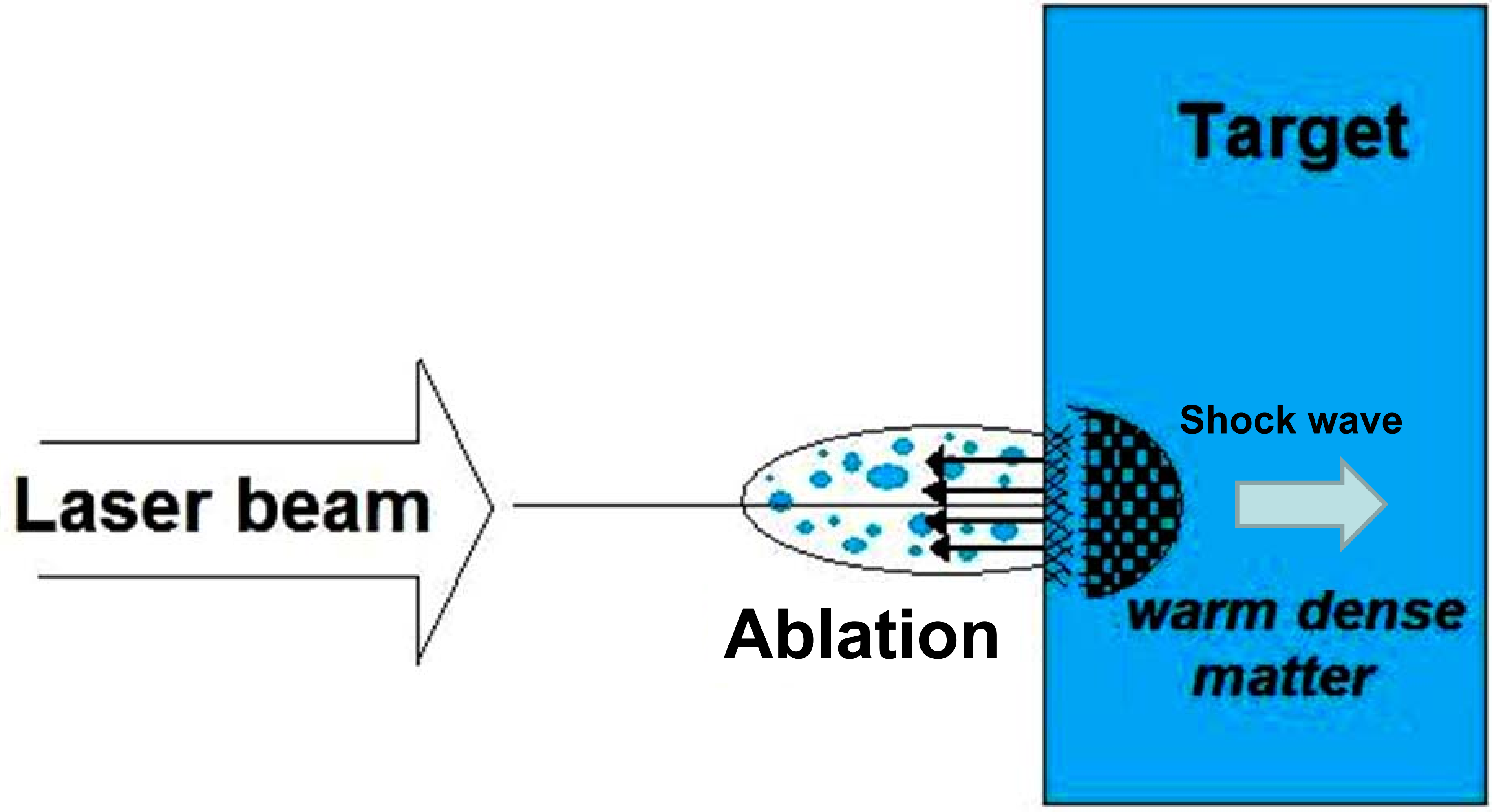
	V_0 , Å^3	E_c , eV	C_{11} , GPa	C_{12} , GPa	T_{melt} , K
experiment	10.22	3.8	202	170	1338
MD	10.23	4.1	225	180	1210

Au isotherms at T_i = 300 K and various temperatures T_e



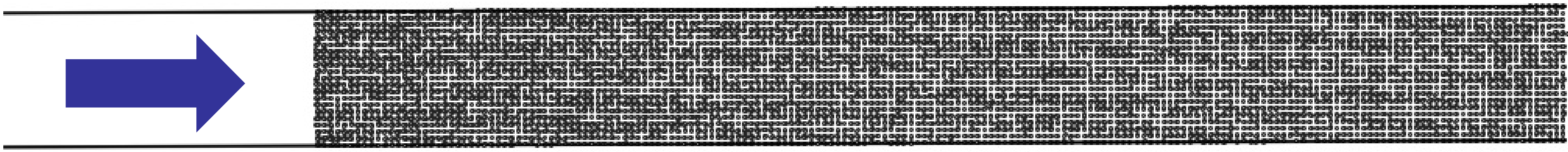
Atomistic simulation of laser ablation of Au

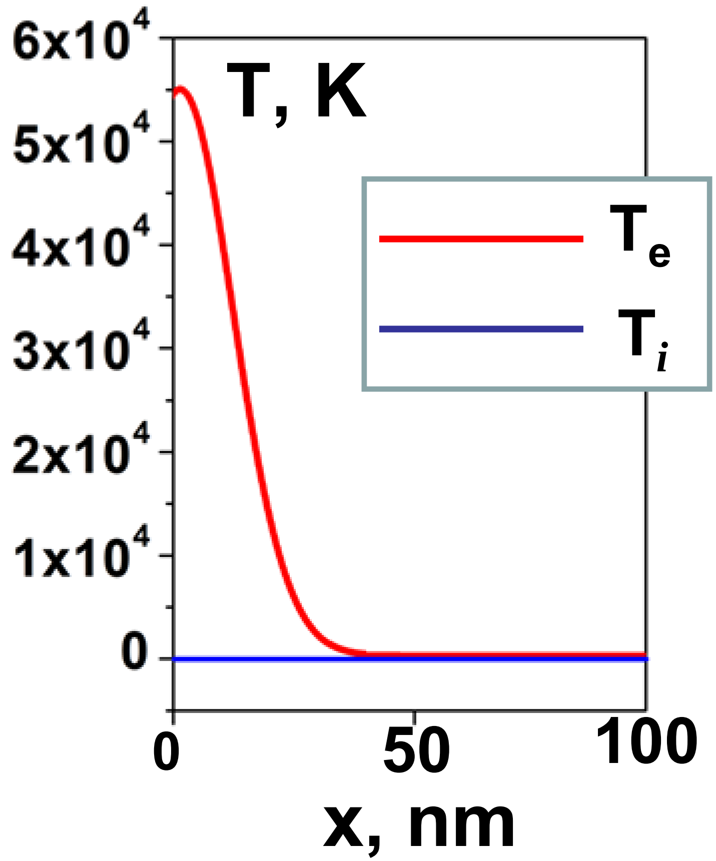
Picosecond laser ablation



2T Atomistic Model of Irradiation

Laser pulse





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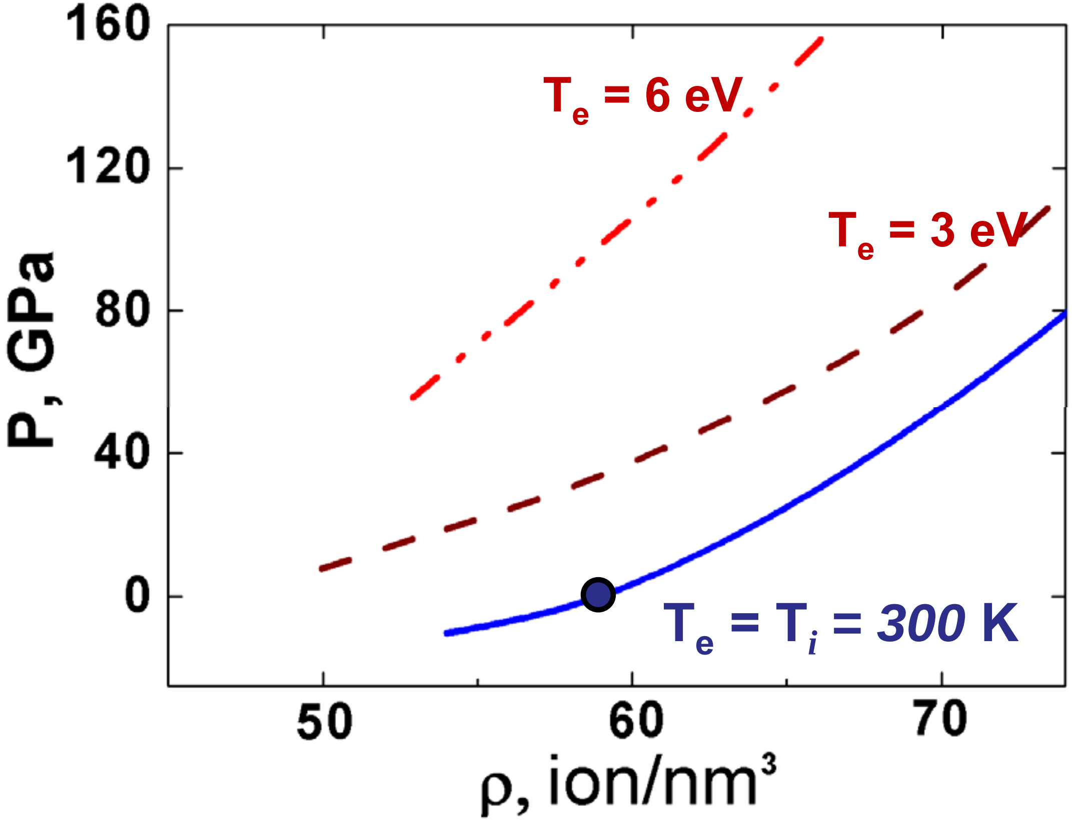
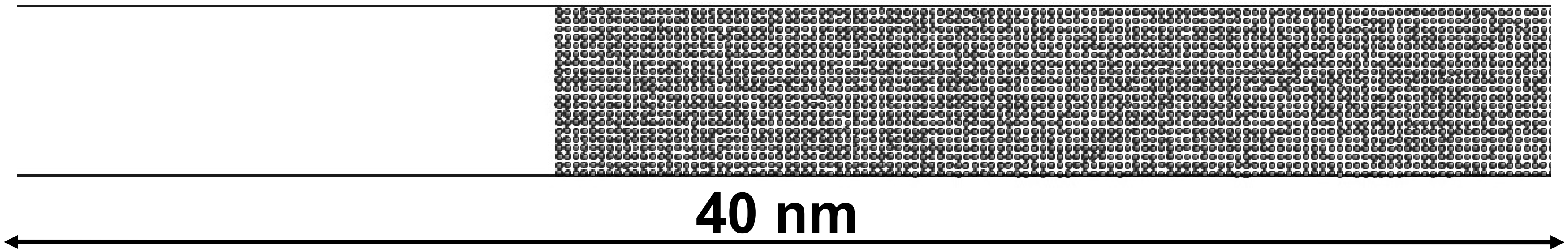
electron temperature dependent (ETD)

- Thermal conductivity equation for electronic subsystem:

$$C_e\frac{\partial T_e}{\partial t} = \nabla\left(\kappa_e\nabla T_e\right) - G_p\left(T_e - T_a\right)$$

Rarefaction wave in 2T media





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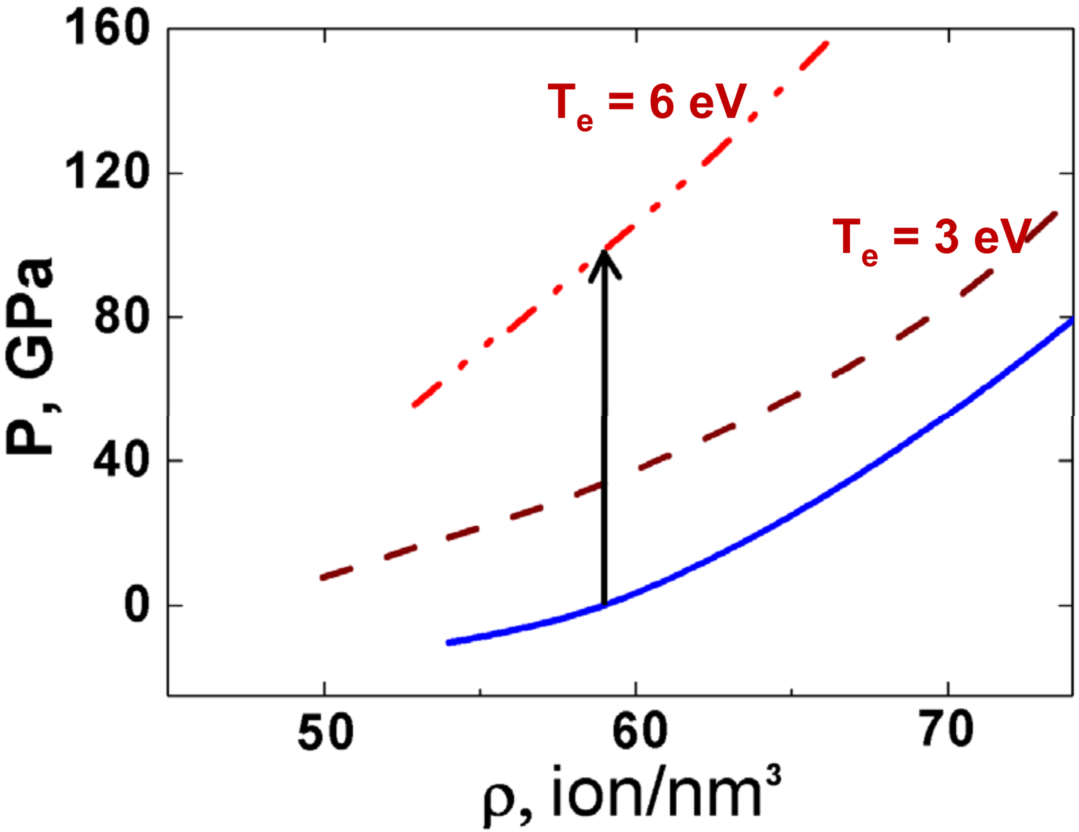

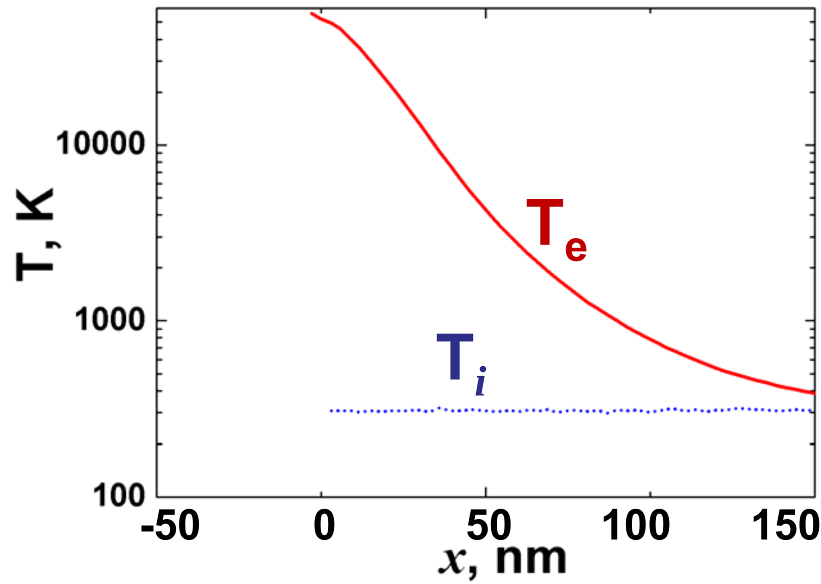

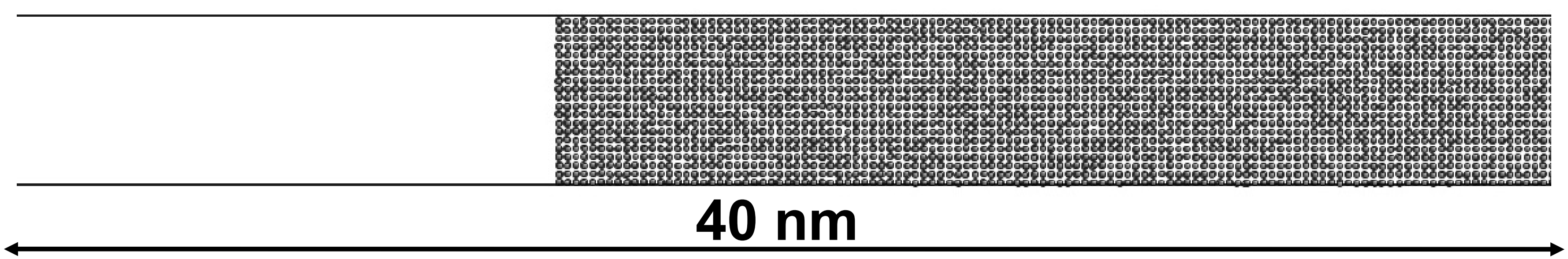

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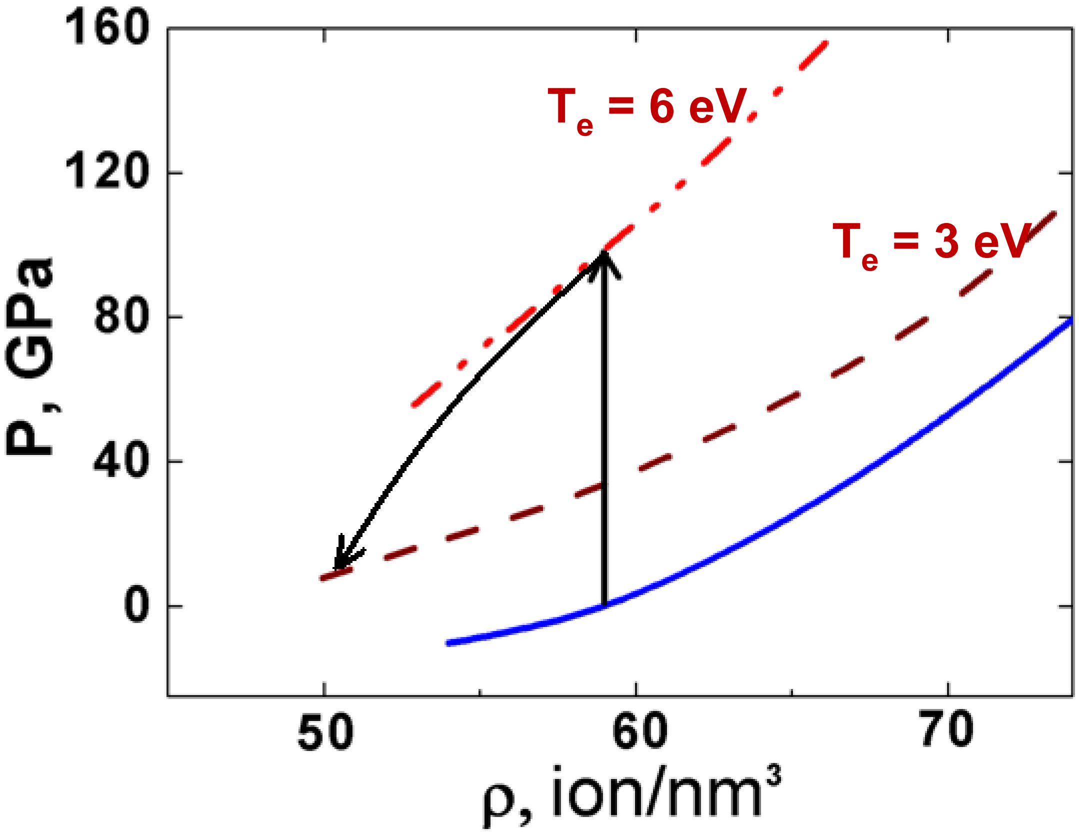
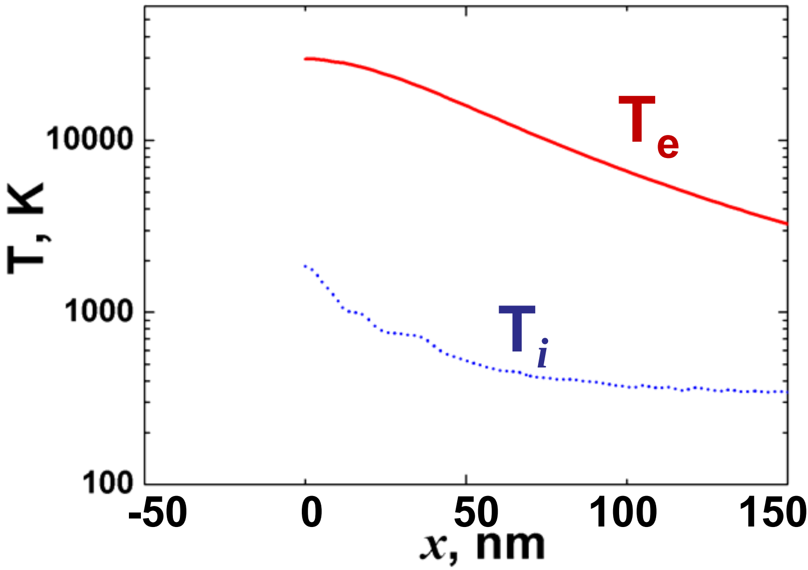
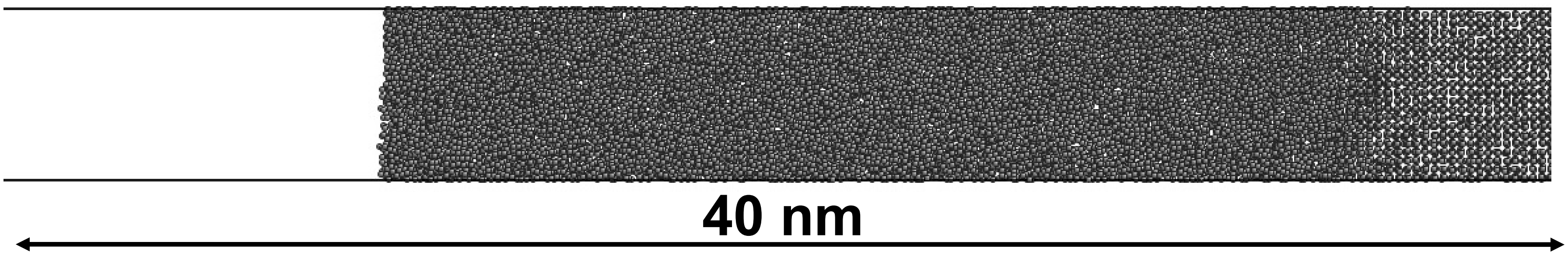
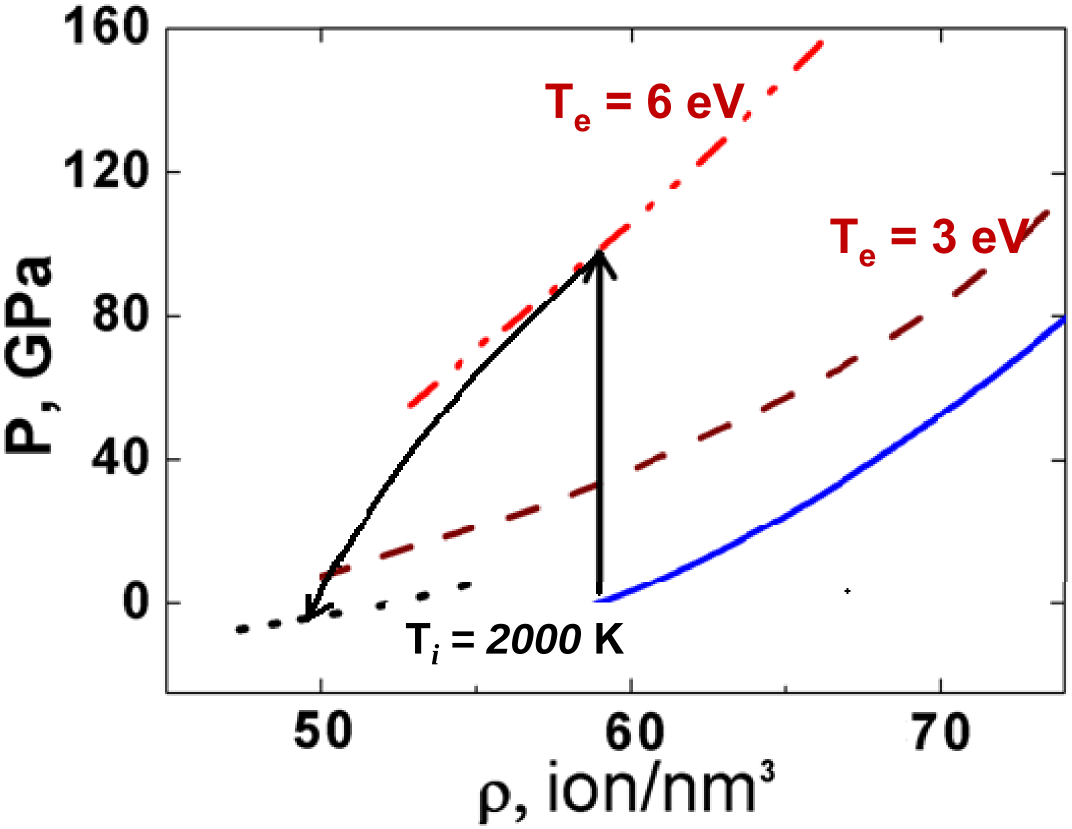
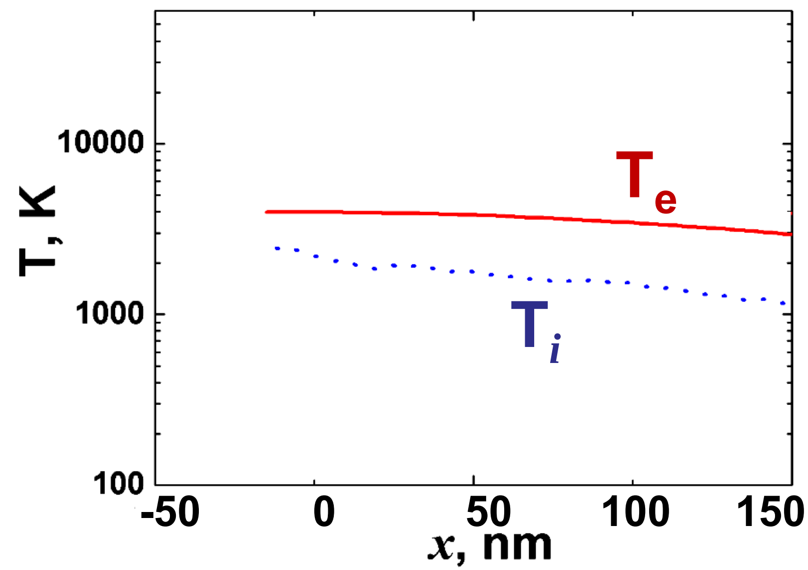


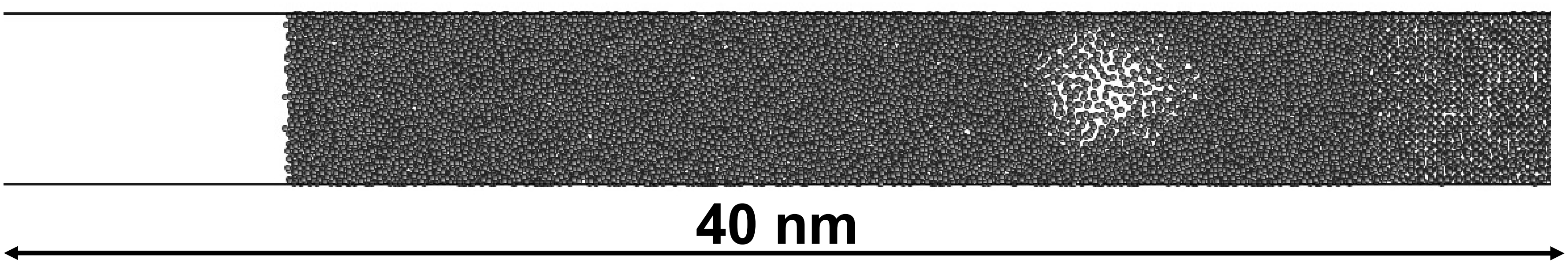




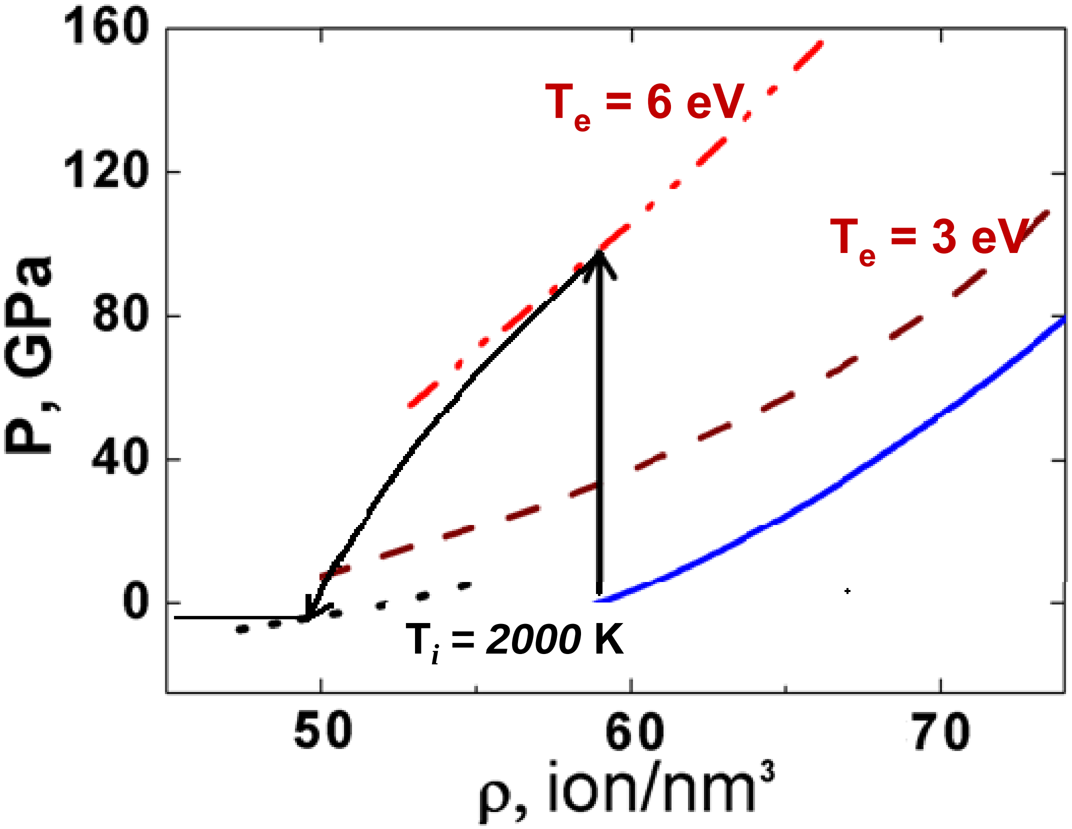
Rarefaction wave in 2T media

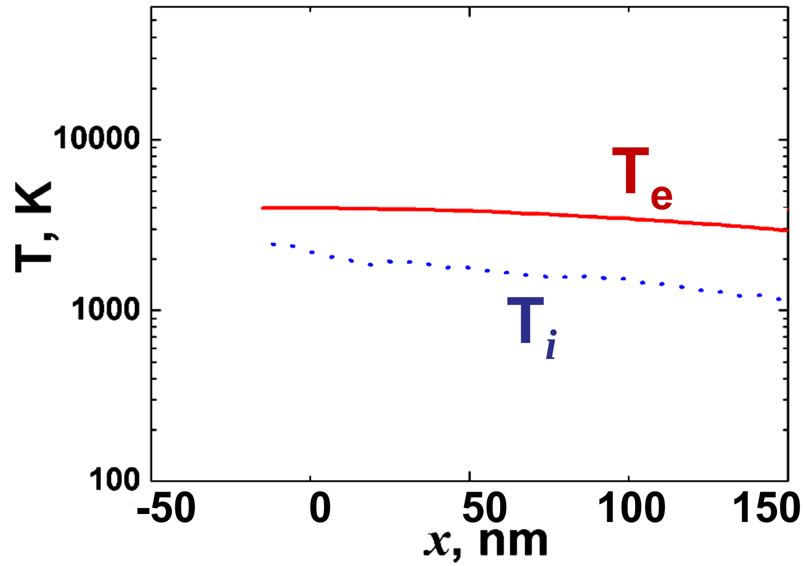


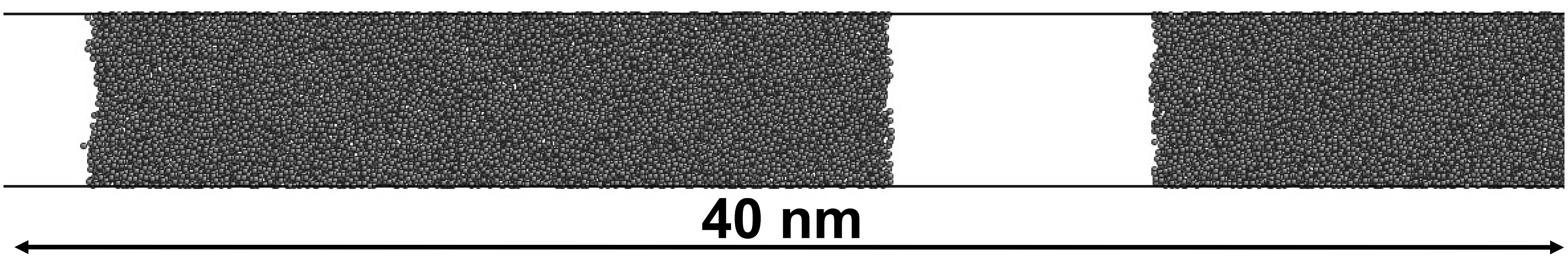




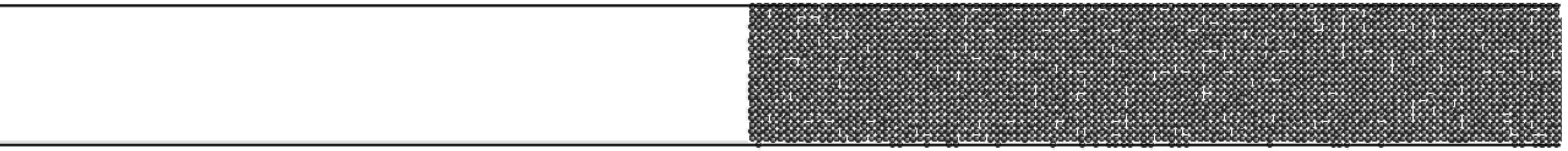
Rarefaction wave in 2T media





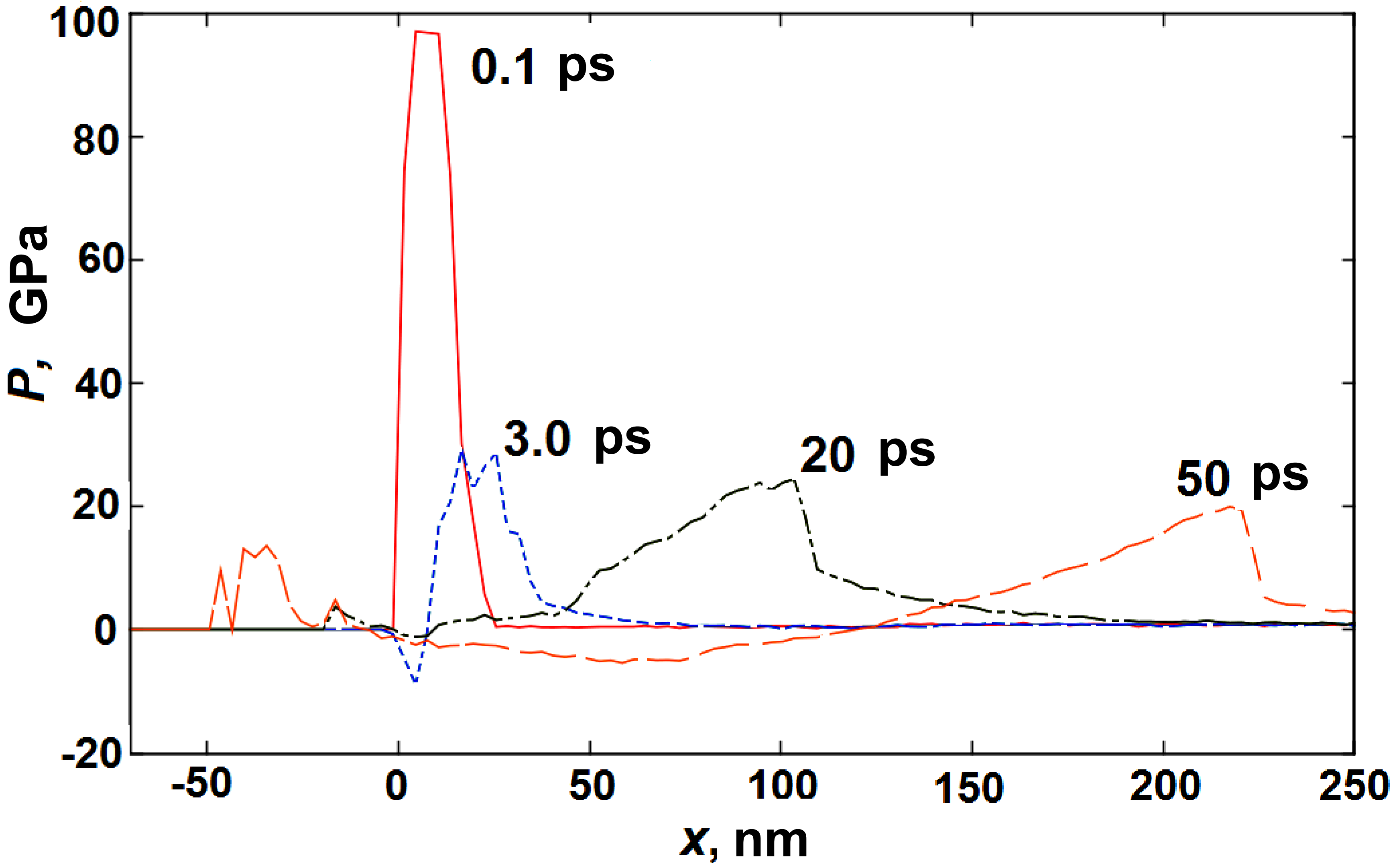


Rarefaction wave in 2T media



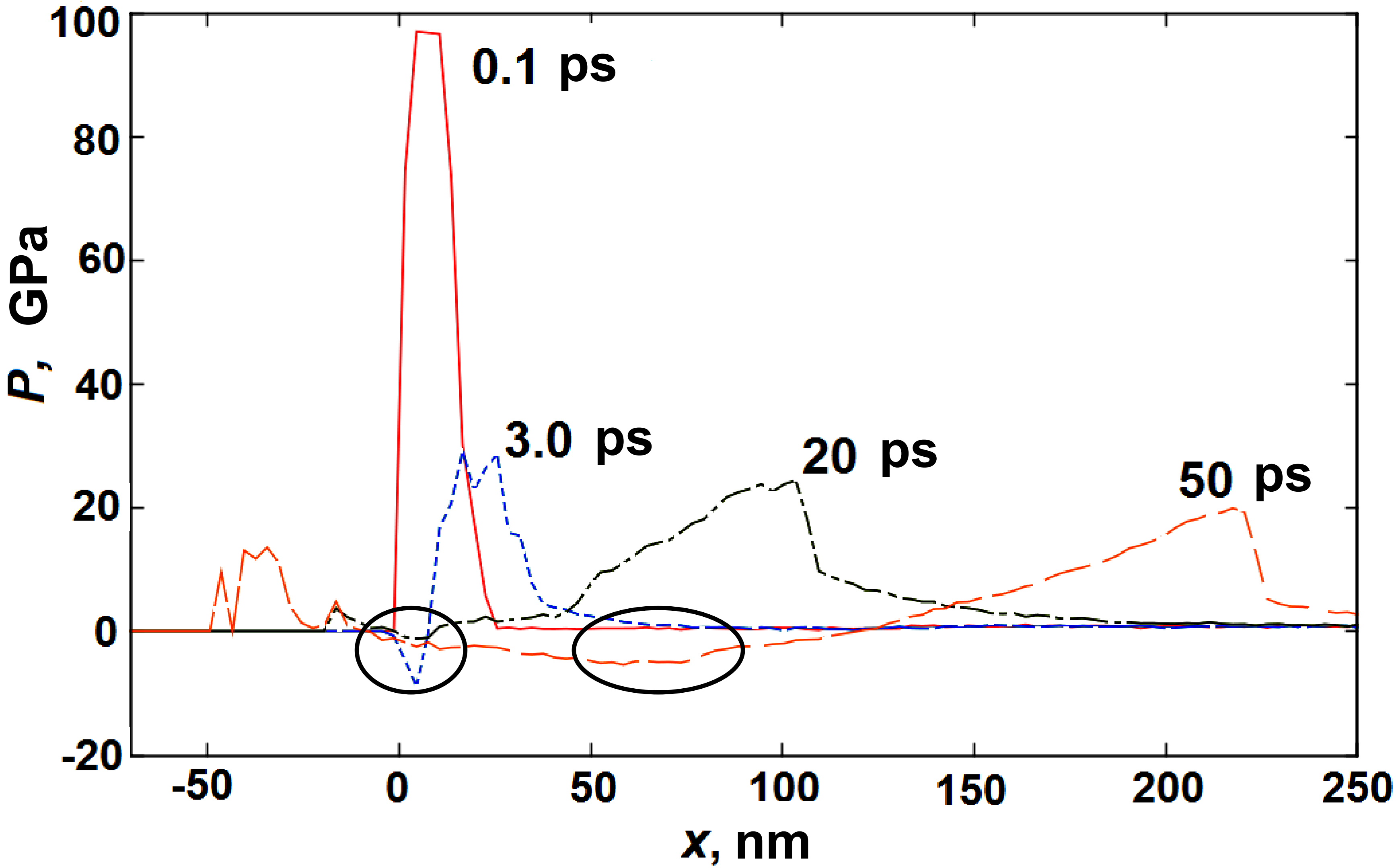
I = 500 J/m² **d = 20 nm**

Ablation on short and long timescales



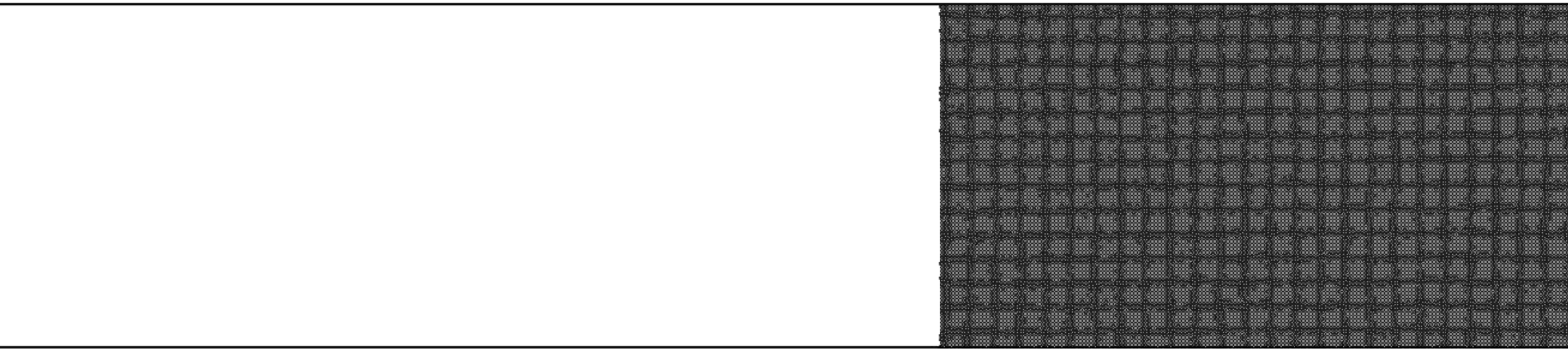
I = 1600 J/m²

Ablation on short and long timescales



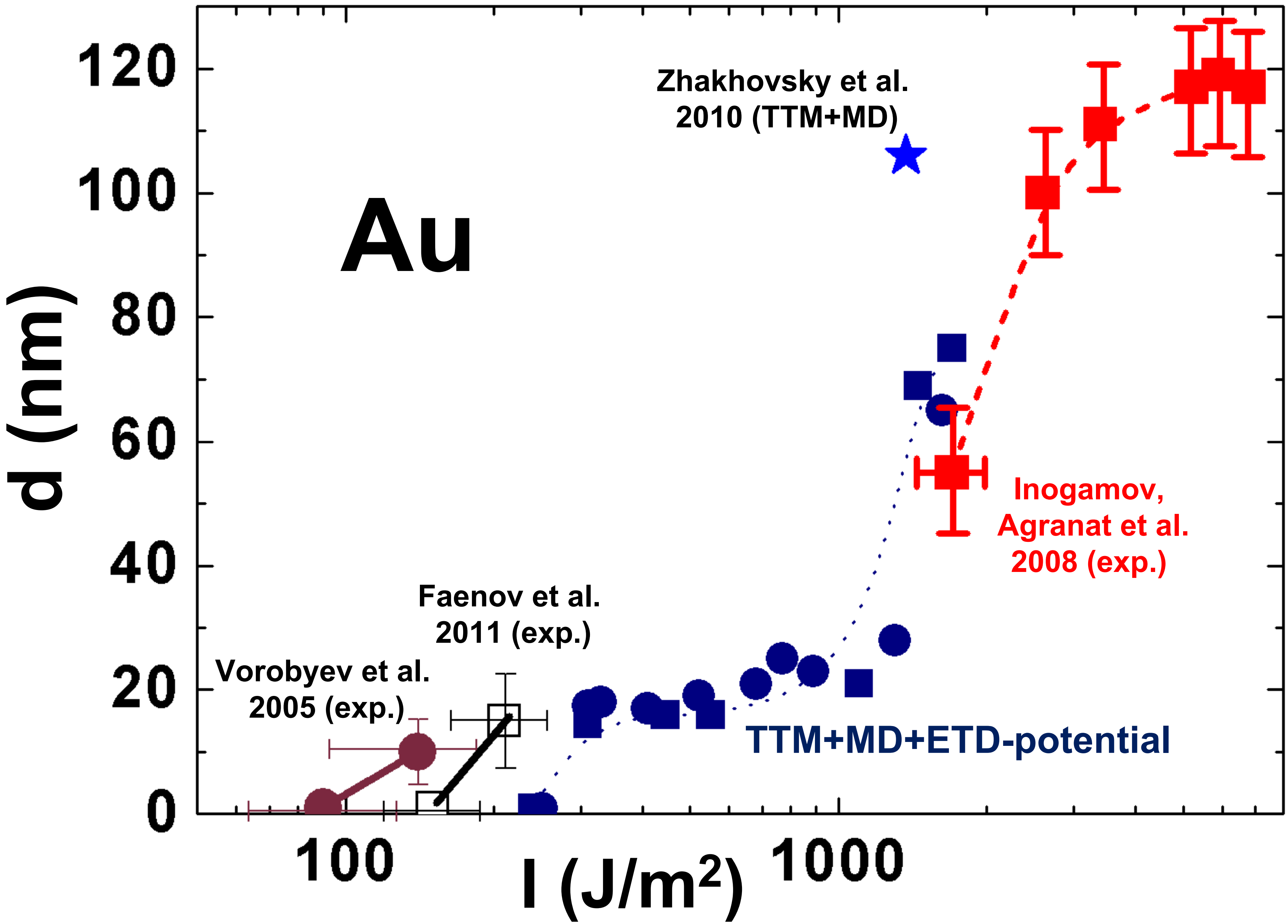
I = 1600 J/m^2

Ablation on short and long timescales



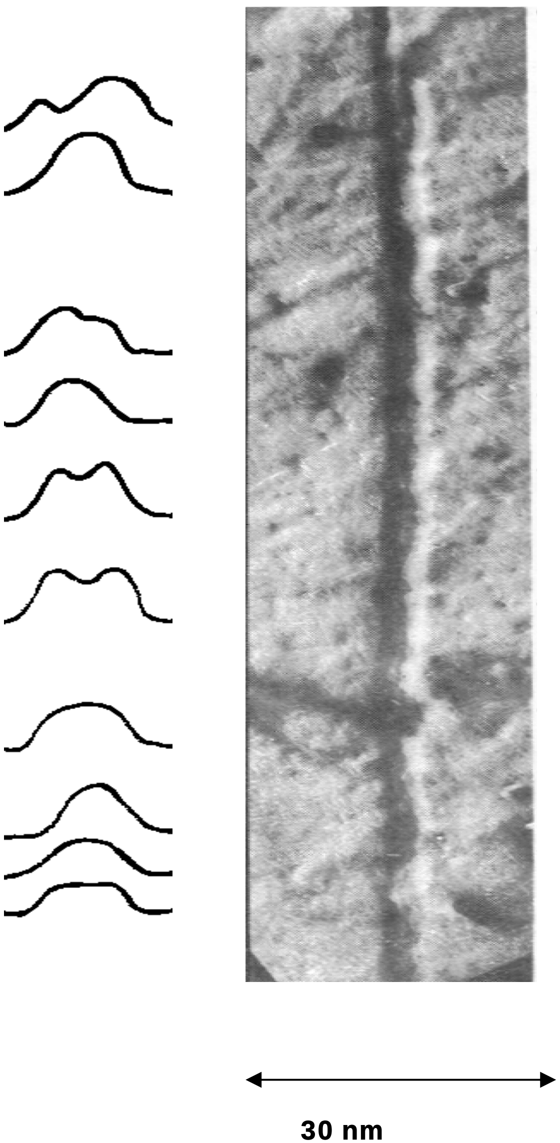
$I = 1600\ J/m^2$

Dependence of crater depth on absorbed fluence



Atomistic simulation
of radiation damage in Mo

Damage produced by fission products

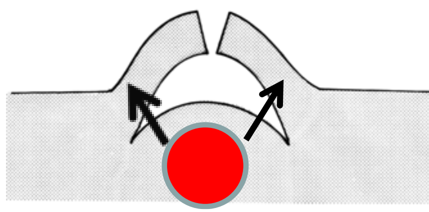


~ 200 MeV/fission

FISSILE NUCLEUS

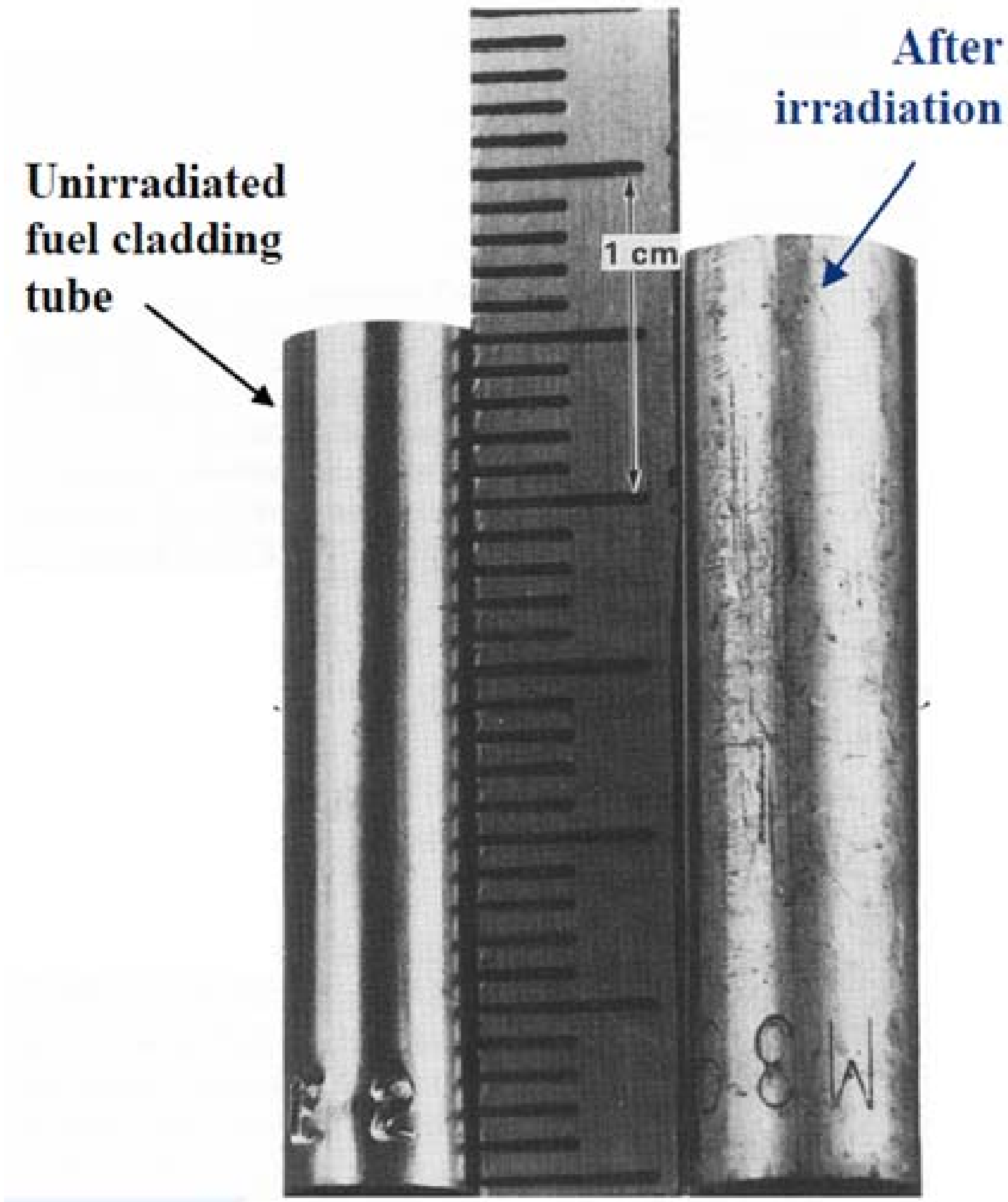
$$n + {}^{235}U \rightarrow {}^{A1}X_1 + {}^{A2}X_2 + \nu\, n + \gamma$$

FISSION PRODUCTS



- **primary radiation damage**
- **clustering of defects**
- **change of the mechanical properties**

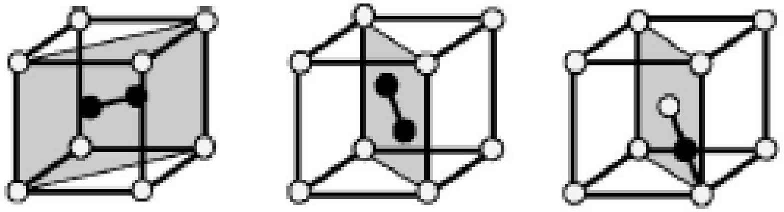
Damage produced by fission products: swelling



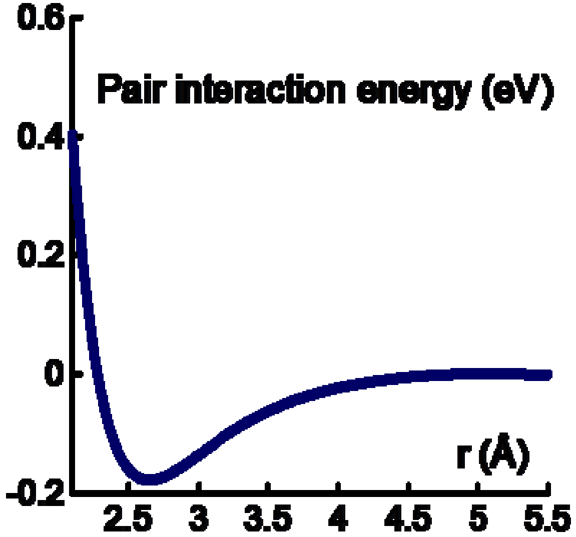
- 20% cold-worked 316 stainless steel tube used for fast reactor fuel cladding.
- Irradiated to ~80 dpa at 510ºC.
- ~33% increase in volume, leading to linear strains of ~10%.
- Swelling in absence of physical constraints is completely isotropic.
- Constrained swelling leads to stresses that generate anisotropic distribution of strains.

Constructing interatomic potentials for Mo-Mo, Mo-Xe, U-U

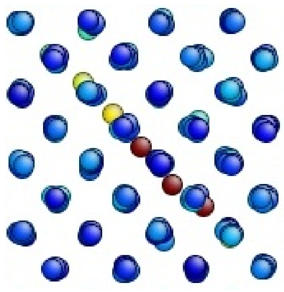
Configuration set
(+ per-atom forces, energies, stresses)

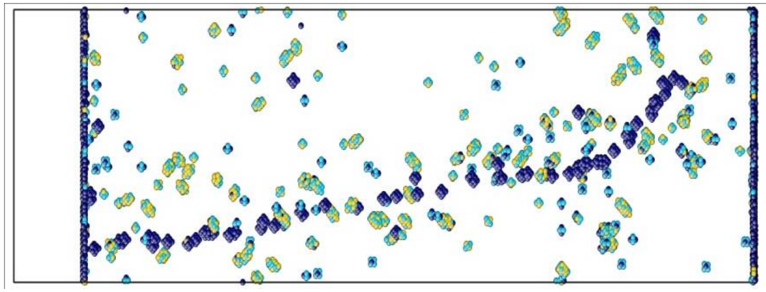


EAM potential

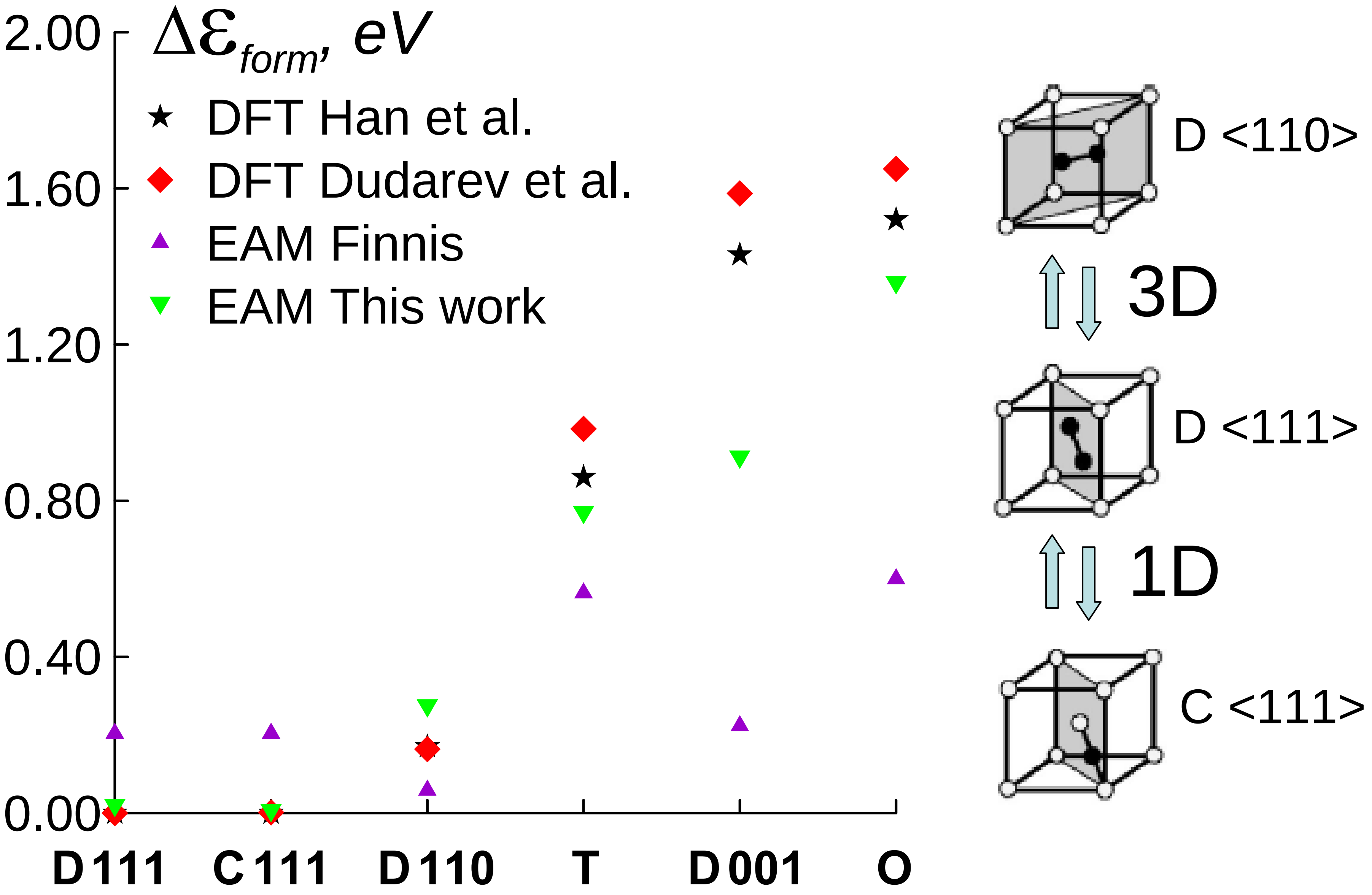


Static and kinetic characteristics

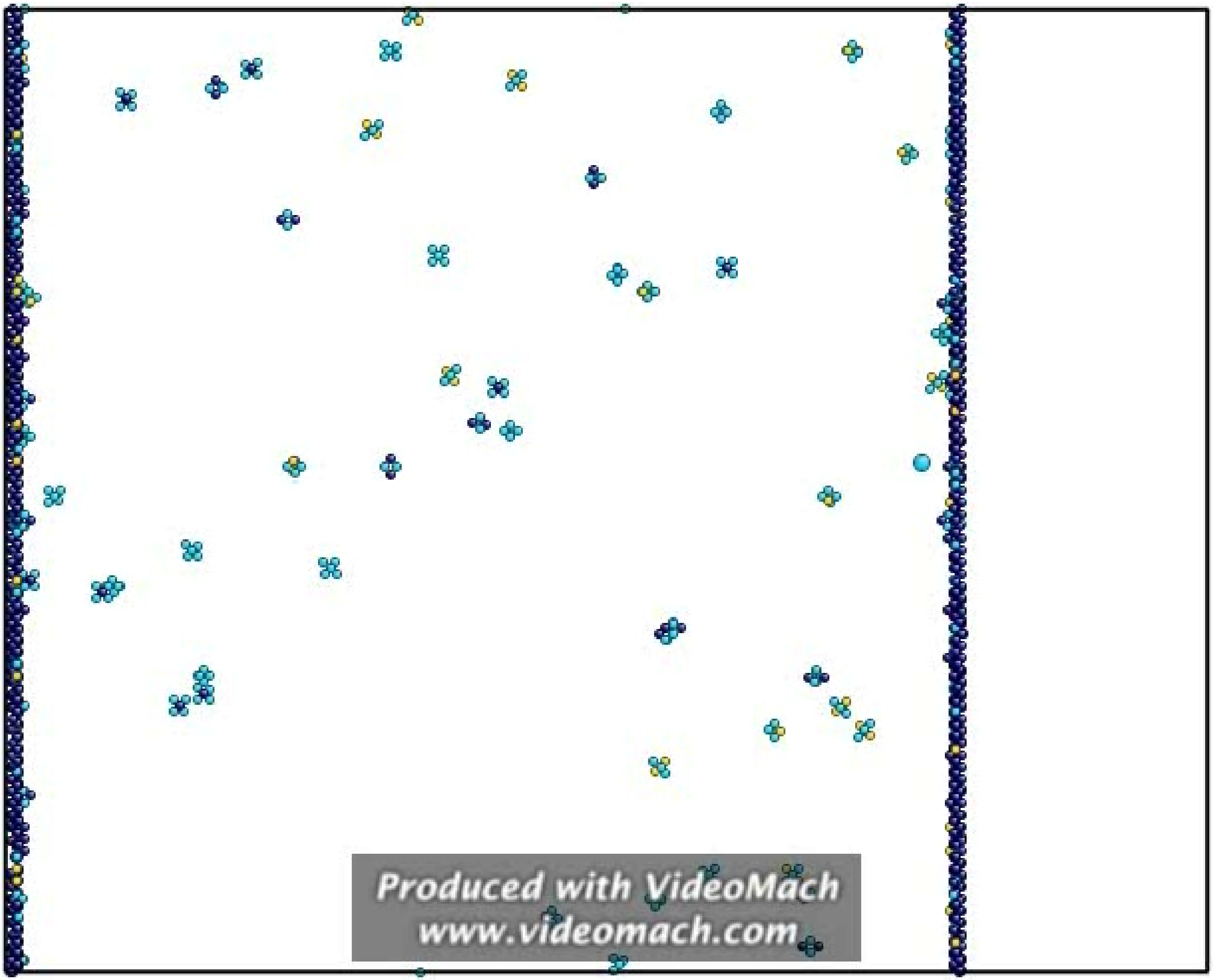




EAM potential for Mo that describes energies of defects



Mo irradiation by Xe ions: evolution of defects

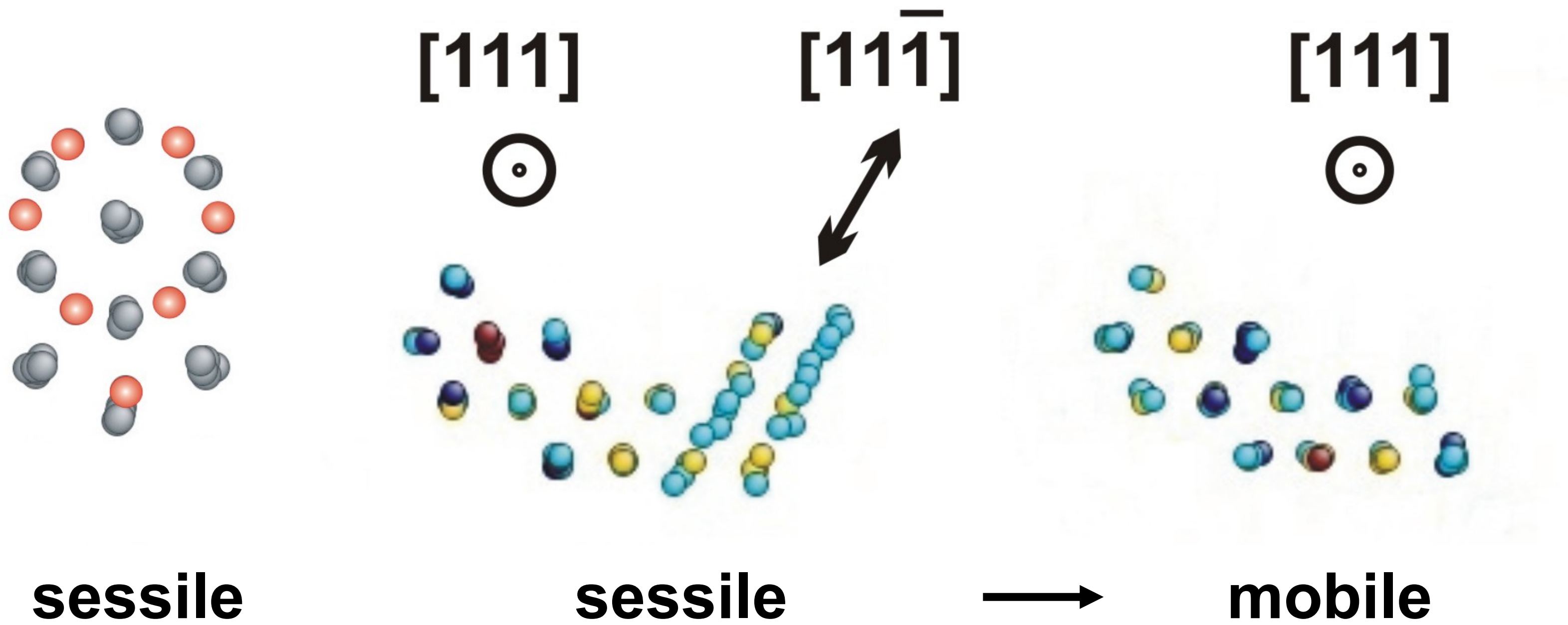


(100) Surface

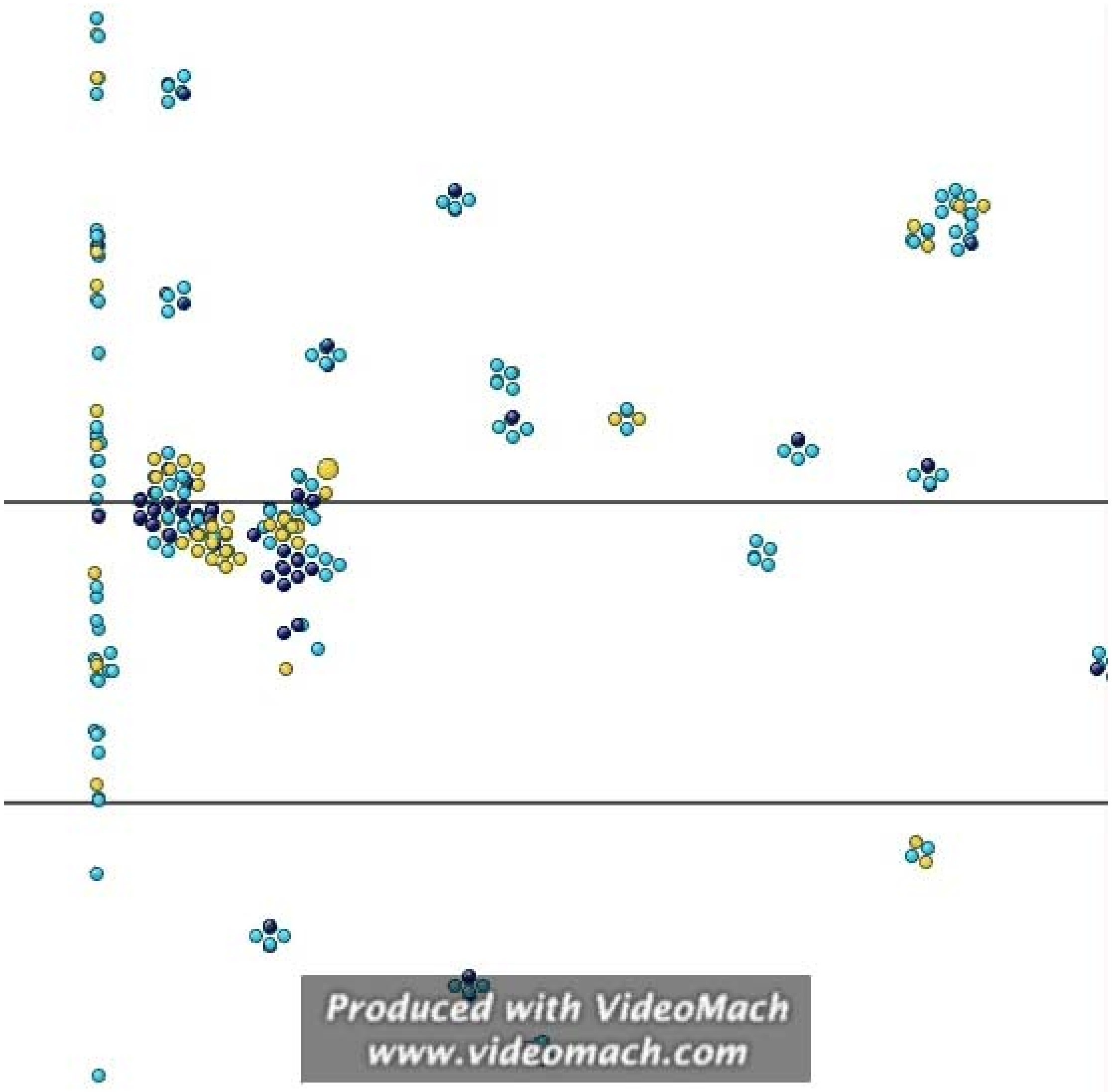
1000 K, 3.16 A
E (Xe) = 42 keV
80x80x80
(Starikov Mo-Xe)

Coordination number

Displacement cascade: Self interstitial atom clusters



Displacement cascade: vacancy dislocation loops



(110) Surface

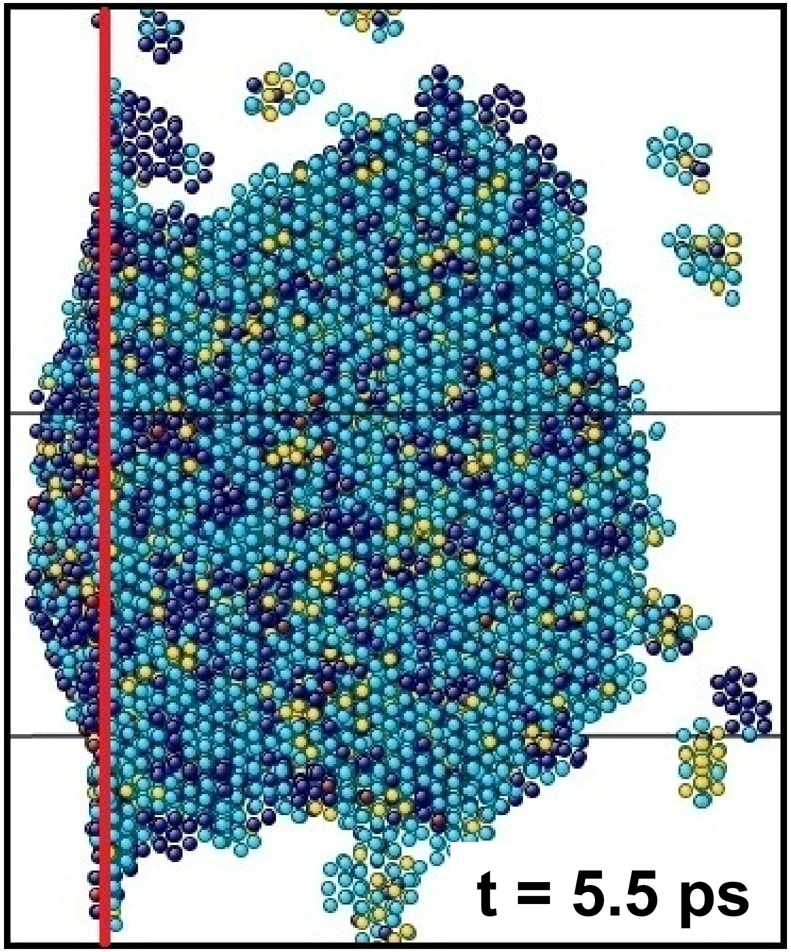
1000 K, 3.16 A
E (Xe) = 42 keV
80x60x60
(Starikov Mo-Xe)

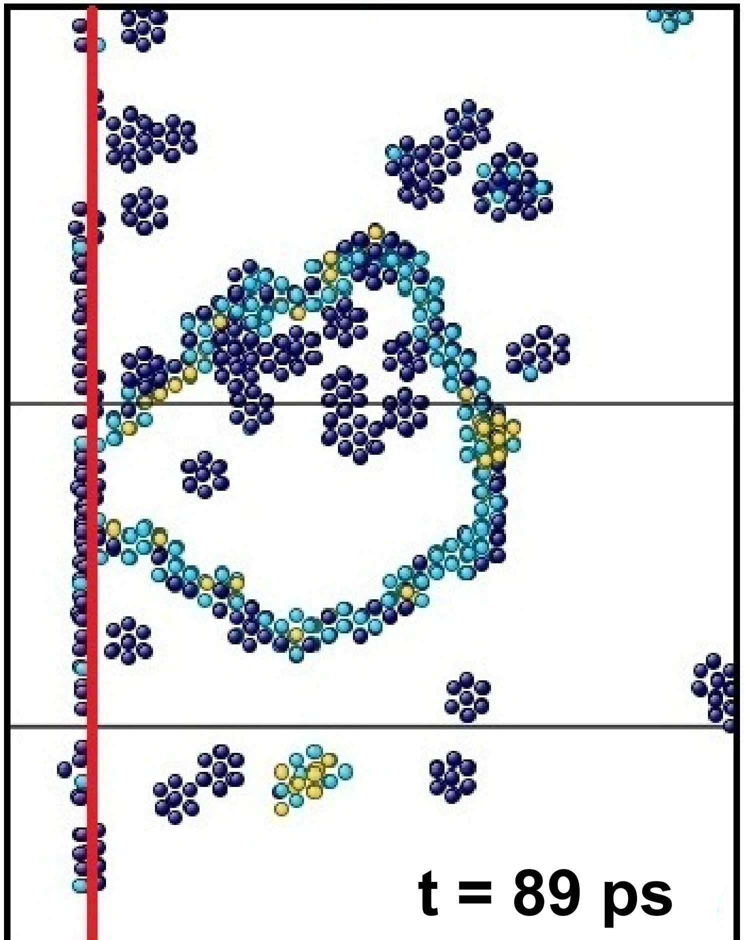
Coordination number

Displacement cascade: vacancy dislocation loops

(110) Surface
80x60x60

1000 K, 3.16 A
E (Xe) = 42 keV
(Starikov Mo-Xe)





Conclusions

1. Electron temperature dependent potential is constructed by force matching to DFT data

2. High electron pressure lead to a faster expansion and ablation at “short” times

3. Dependence of ablation depth on absorbed fluence: self-consistent description of different experiment is achieved

4. Mo foils under Xe irradiation: vacancy dislocation loops formation near the surface

5. Increase of the ion mass lead to an increased of the defect yield