4th EMMI workshop on Plasma Physics with Intense Heavy Ion and Laser Beams

May 02 – 04, 2011, GSI, Darmstadt, Germany

Formation and mobility of clusters of defects in metals under ion irradiation

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1. Molecular dynamic (MD) models
2. Construction of the potential for MD
3. Defect energies and mechanisms of diffusion
4. Formation of defects in displacement cascades under ion irradiation

1. Molecular dynamic (MD) simulations: aims and models

Displacement cascade produced by ion

Evolution of the material microstructure

- production, clustering, growth of defects
- plastic deformation
- formation of voids and bubbles
- phase transitions

Change of the mechanical properties of material

- radiation hardening/softening
- swelling, fracture, spall

Specific questions discussed

mechanisms of production of clusters of defects and dislocation loops, effect of impurities

the effect of ion mass on the defect yield: beyond the NRT standard

the influence of surfaces: ablation, spall

role of the thermal spike stage in defect production

the mobility of self interstitial atoms (SIAs) and clusters, dislocation loops

Two-temperature model: MD for ions + electronic subsystem

- MD for atoms + thermostat due to electrons

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

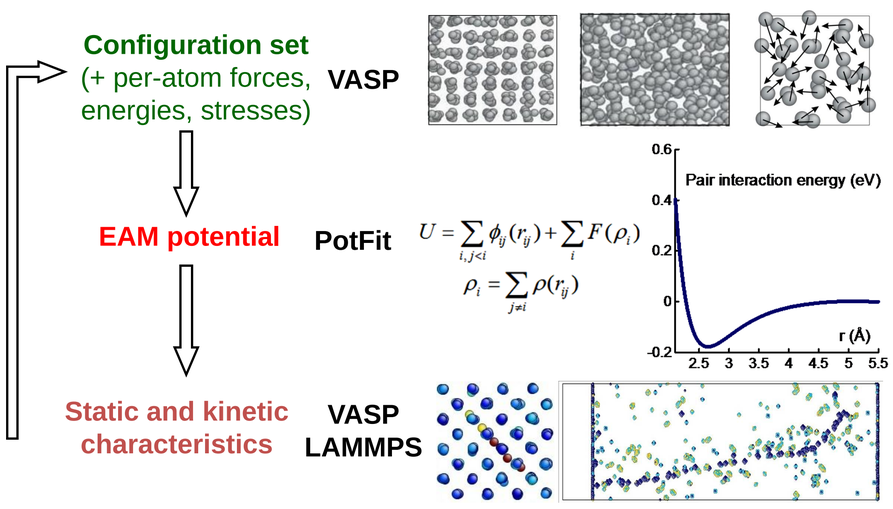
- Interatomic potential with attention to energies of defect structures

- Thermal conductivity equation for electronic subsystem

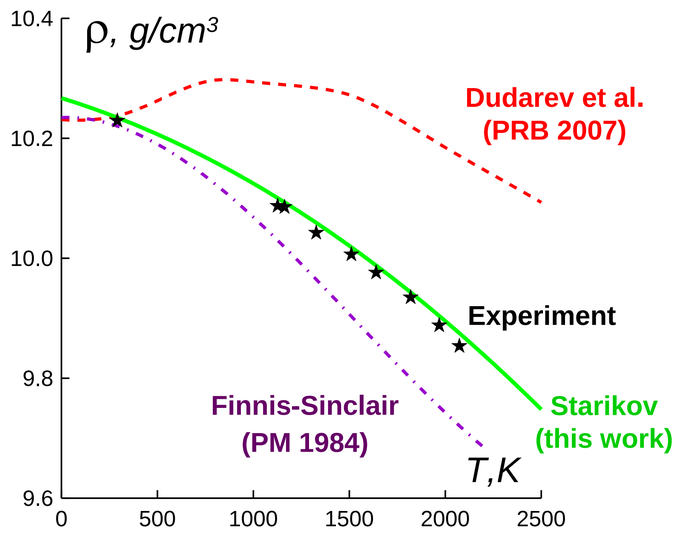
$$C_e\frac{\partial T_e}{\partial t} = \nabla\left(\kappa_e\nabla T_e\right) - G_p\left(T_e - T_a\right)$$

2. Construction of the interatomic potential for Mo-Xe by force matching to *ab initio* data

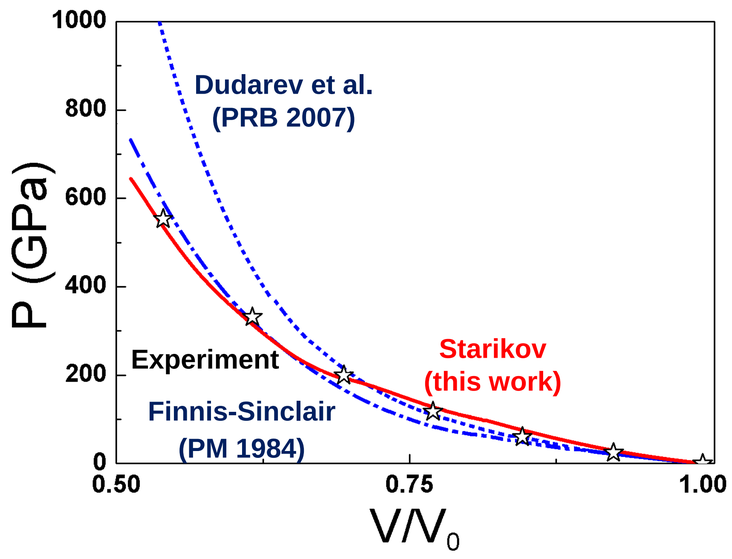
A procedure consisting of fitting the parameters of the new potential (a), testing it to reproduce certain properties (b) and recalculating the starting configuration set with this new potential (c) is performed in an iterative manner in order to provide good description of the desired properties (such as defect formation energies, elastic moduli).



Description of thermal expansion of Mo



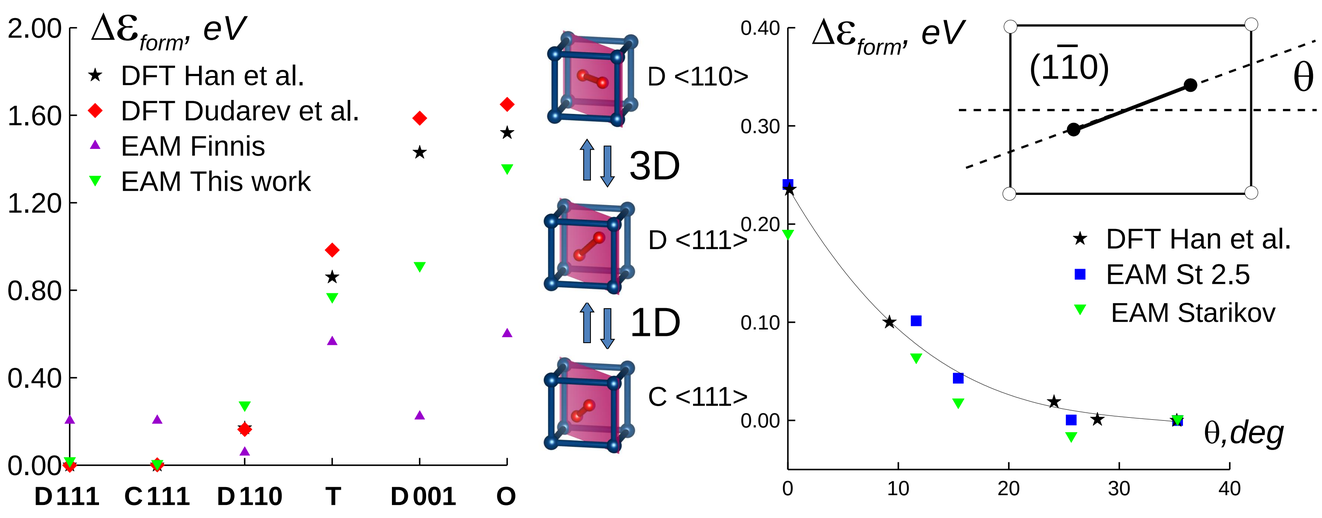
Description of compressibility of Mo at room temperature



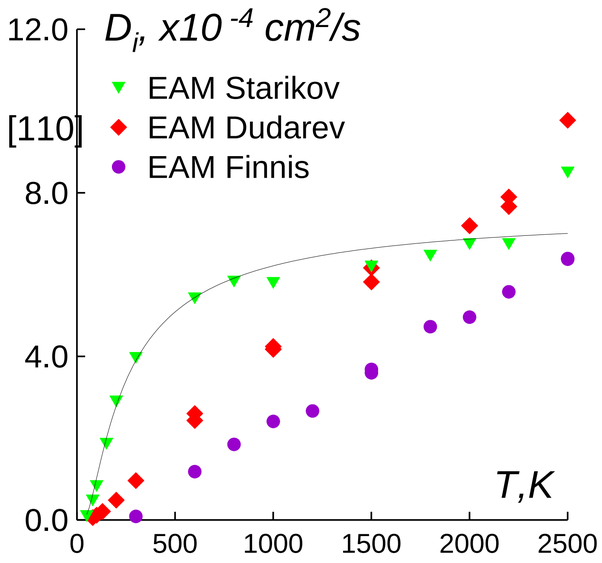
3. Correct description of defect energies and mechanisms of diffusion

A very small difference between SIA configurations D and C along 111 direction provides 1D migration of SIAs at very low temperatures in agreement with the resistivity recovery measurements following electron irradiation.

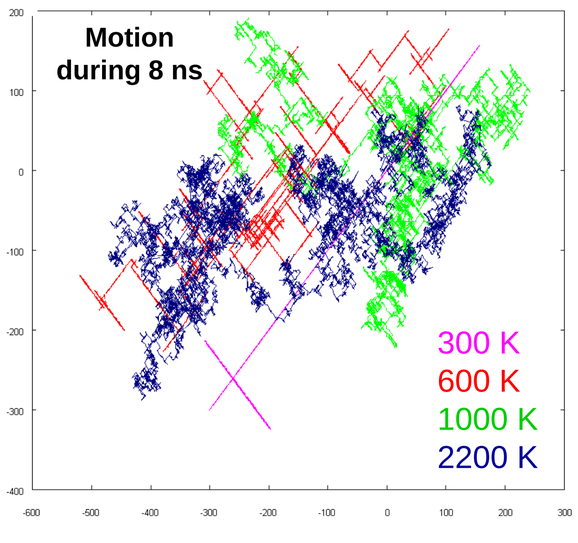
As temperature increases the D111-D110 dumbbell transitions are activated providing rotations of crowdion propagation directions and activation of 3D diffusion.



Temperature dependence of diffusion coefficient of self-interstitial atoms in Mo



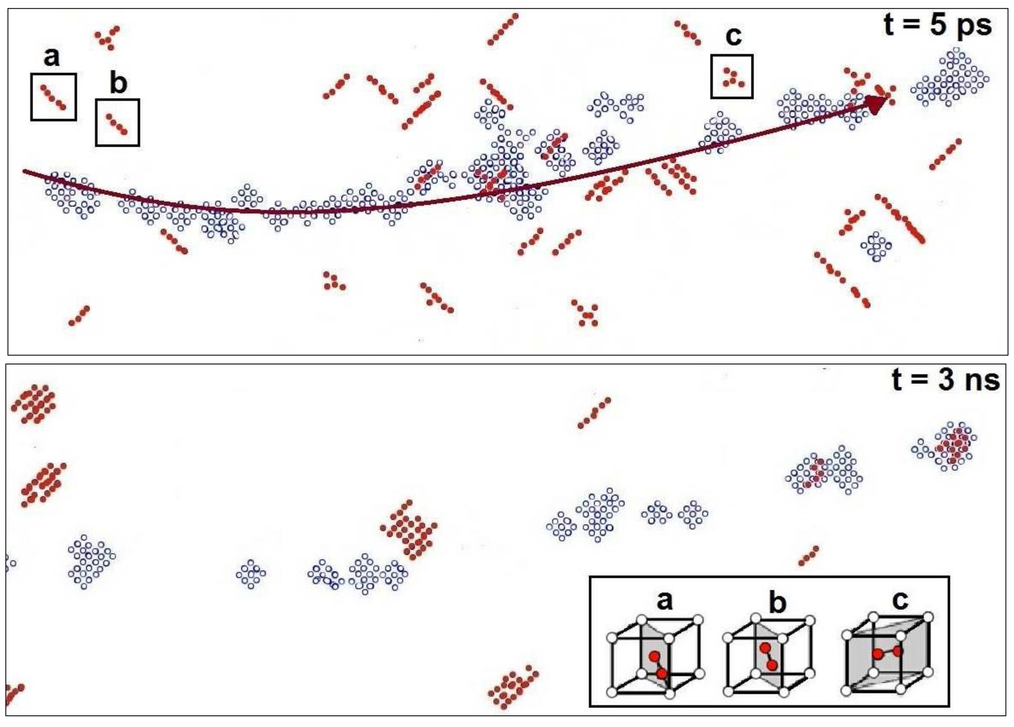
Trajectories of SIA motion in Mo at different temperatures



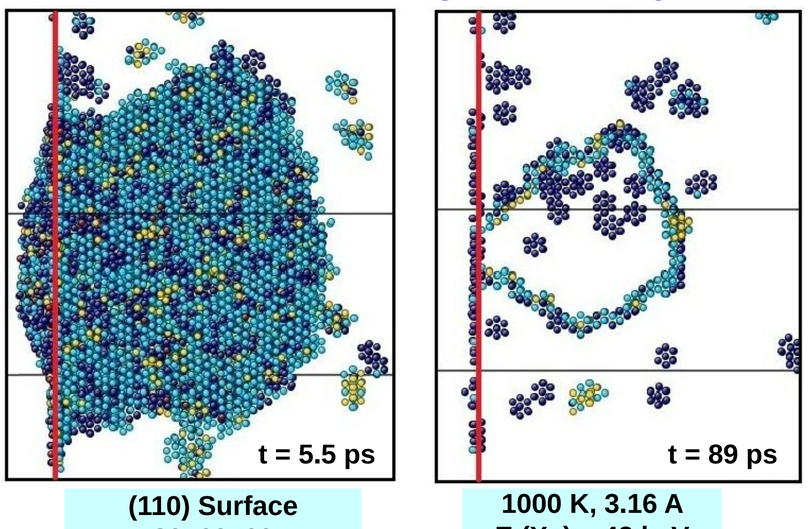
4. Formation of defects in displacement cascades under ion irradiation

Formation of clusters as a result of SIA diffusion to each other and aggregation

A long time is required.
A lot of mobile clusters can be lost on the free surfaces due to their fast migration.
So it is active in the bulk material, e.g. neutron irradiation.



Formation of large vacancy clusters close to the surface during fast cooling



(110) Surface
80x60x60

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

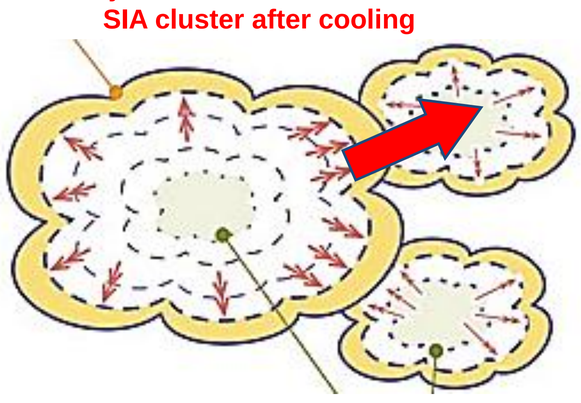
If the energy density deposited by ion in the vicinity of surface is high enough for melting than spontaneous nucleation of large vacancy dislocation loop is possible as a result of fast cooling.

Thus a nature of the dislocation loops observed agrees well with the experiments on ion irradiation of Mo foils [English and Jenkins, Philosophical Magazine 90. 821. 2010.]
Enhanced production of the loops for molecular ions (at the same energy per ion) than can be connected to the smaller penetration depth of molecular ions in comparison to single ions.

The mobility of segments of the vacancy dislocation loop is high, however the motion of the entire loops is strongly hindered by a number of point defects in the region it have been produced. Thus it lead to a reduced mobility of such loops and their preferential survival. Depinning of the loop is observed due to an external stress field in the proximity to free surface of favorable orientation.

Formation of large SIA and vacancy clusters due to interaction of subcascades

Injection of atoms result in SIA cluster after cooling



Low density regions in the cores of subcascades

Several mechanisms for injection of atoms during subcascades interaction are possible:

a) flow in a liquid phase induced by an expanding internal cascade
b) meeting of the main and secondary supersonic shock waves with high atomic density at their fronts and low density disorder behind [Calder et al. Philosophical Magazine 90. 863. 2010.]
c) dislocation punching [de la Rubia and Guinan, Phys. Rev. Lett. 66. 2766. 1991.]

However, for Mo irradiation by Xe interstitial clusters produced directly in the cascade are quite small (2-4 SIAs). No evidence of large SIA clusters formation on the early stage of cascade as described in above for Fe are found.

Simulations were carried out on the computing cluster MIPT-60 of the Moscow Institute of Physics and Technology.

This work was supported in part by the U.S. Dept. of Energy Office of Advanced Scientific Computing Research, Office of Science, under Contract DE-AC02-06CH11357, by the Program for Basic Research of the RAS No. 2, RFBR 09-08-01116 grant and president's grant MK-3174.2011.8.