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MD simulation of interaction between radiation damages and microstructure: voids, helium bubbles and grain boundaries

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MD simulation of interaction between radiation damages and microstructures: voids, helium bubbles and grain boundaries

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Collaboration

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Motivation

Rate theory

J. L. Katz, H. Wiedersich, J. Chem. Phys. 55 (1971) 1414-1425

A. D. Brailsford, R. Bullough, J. Nucl. Mater. 44 (1972) 121-135

$$dC_i/dt = G_i - \alpha_{iv}C_iC_v - \kappa_i D_i C_i + \nabla\left(D_i\nabla C_i + \frac{D_iC_i}{kT}\nabla U_i\right) \qquad \kappa_i = \sum_j \kappa_i^j$$

$$dC_v/dt = G_v - \alpha_{iv}C_iC_v - \kappa_v D_v C_v + \nabla\left(D_v\nabla C_v + \frac{D_vC_v}{kT}\nabla U_v\right) \qquad \kappa_v = \sum_j \kappa_v^j$$

j = voids, dislocations, grain boundaries etc

$$D_{i,v} = D_{i,v}^0 \exp(-E_{i,v}/kT) \qquad \alpha_{iv} = 4\pi r_{iv}(D_i + D_v)$$

It is assumed that under irradiation, Frenkel pairs of vacancies and SIAs are created in the bulk and annihilated at extended defects, such as dislocations, grain boundaries, cavities and the like, which are thus considered primarily as the ***sinks*** for point defects. However, extended defects can act also as the ***radiation-induced sources*** of point defects, which can result in a new driving force of the microstructural evolution.

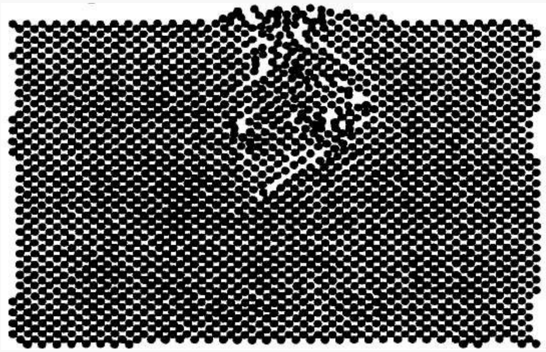
Motivation

Favored formation of vacancies close to extended defects observed by simulation of collision cascade development near

External surface

10 keV, Au

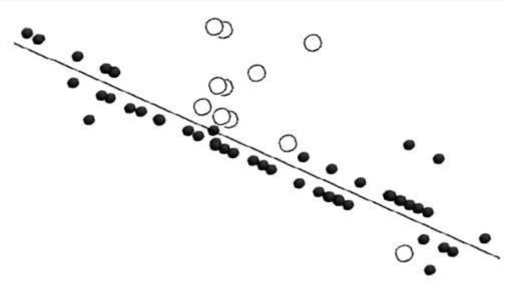
M. Ghaly and R.S. Averback, Phys. Rev. Lett. 72 (1994) 364.



Bilayer interfaces

5 keV, Co/Cu

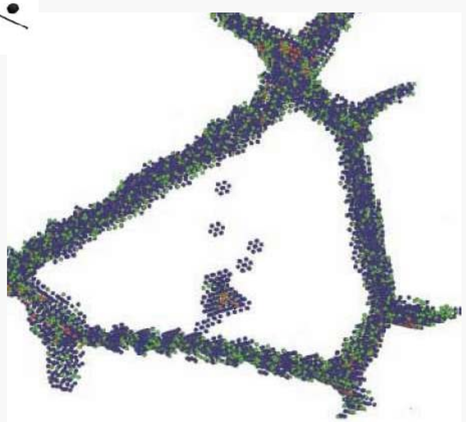
K. Nordlund and R. S. Averback, Phys. Rev. B59 (1999) 20.



Grain boundaries

20 keV, Ni

M. Samaras, P. M. Derlet, H. Van Swygenhoven, M. Victoria, Phys. Rev. Lett. 88 (2002) 125505.



Motivation

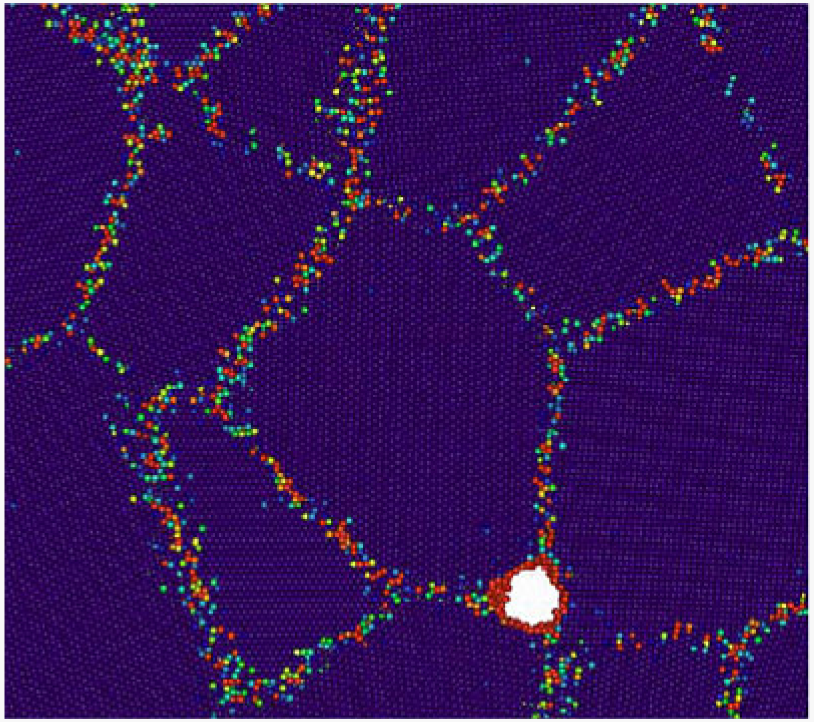
Kai Nordlund et al, Nature 398 (1999) 6722

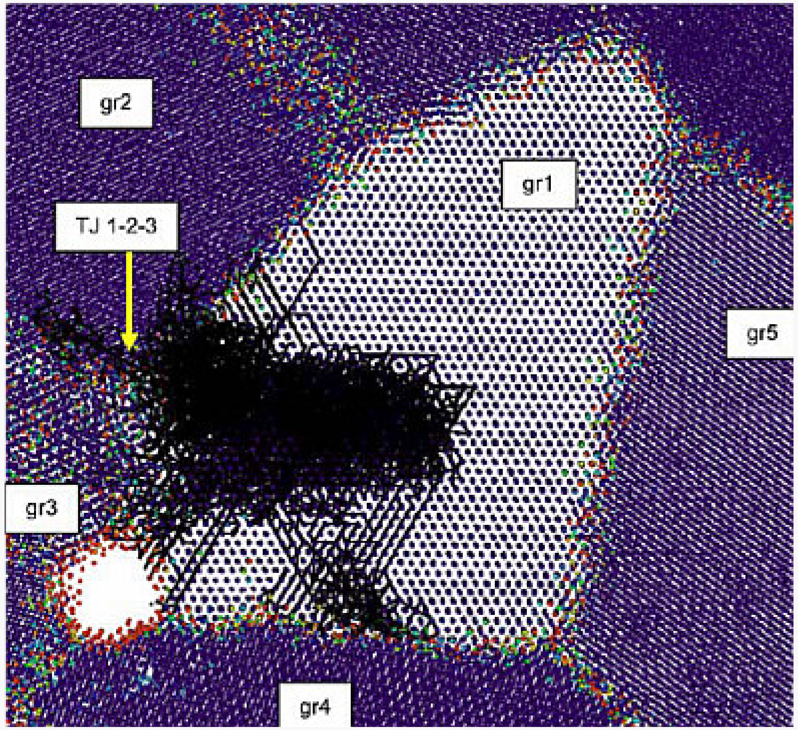
Damage production in bulk and surface events:

	Vacancies		Interstitials	
	Ave.	Max	Ave.	Max
Cu bulk.	32 ± 7	59	35 ± 11	77
Cu surf.	240 ± 50	388	32 ± 9	77
Ni bulk	26 ± 12	71	31 ± 7	57
Ni surf.	38 ± 6	52	27 ± 6	56

Motivation

M. Samaras, W. Hoffelner, M. Victoria, J. Nucl. Mat. 352 (2006) 50–56





Simulation of a pre-existing void in nc bcc Fe indicates that the void plays a role as a sink to self interstitial atoms during displacement cascades.

Outline

- Defect production close to voids in Cu at low energy cascades
- Diffusion and primary damages in Fe
- Biased defects creation near voids in Fe at high energy cascades
- Simulation of point defects production near helium bubbles
- Recrystallization processes under irradiation

Simulation method

Molecular Dynamics with Empirical force-field

EAM potential: $$U = \sum_{ij} V(r_{ij}) + \sum_{i} F(\overline{\rho}_i) \,, \qquad \overline{\rho}_i = \sum_{j} \phi(r_{ij})$$

Parameterization:

Cu: **Yu. Mishin et al, Phys. Rev., B 63 (2001) 224106.**

Fe: **M.I. Mendelev et al, Phil. Mag. 83 (2003) 3877–94.**

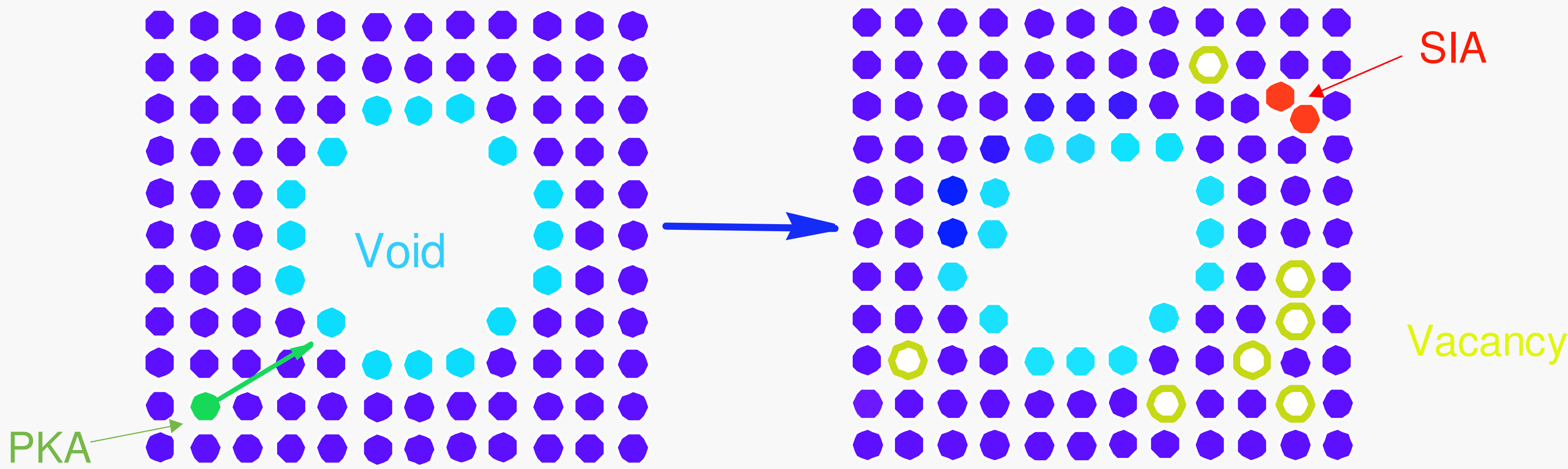
He: **D.E. Beck D.E. Mol. Phys. 14 (1968) 311.**

Fe–He: **N. Juslin, K. Nordlund, J. Nucl. Mater. 382 (2008) 143.**

Defect production close to voids in Cu

N. P. Lazarev, V. I. Dubinko, Radiat. Eff. & Def. Solids 158 (2003) 803.
V.I. Dubinko, N.P. Lazarev, Nucl. Instr. Meth. Phys. Res. B 228 (2005) 187

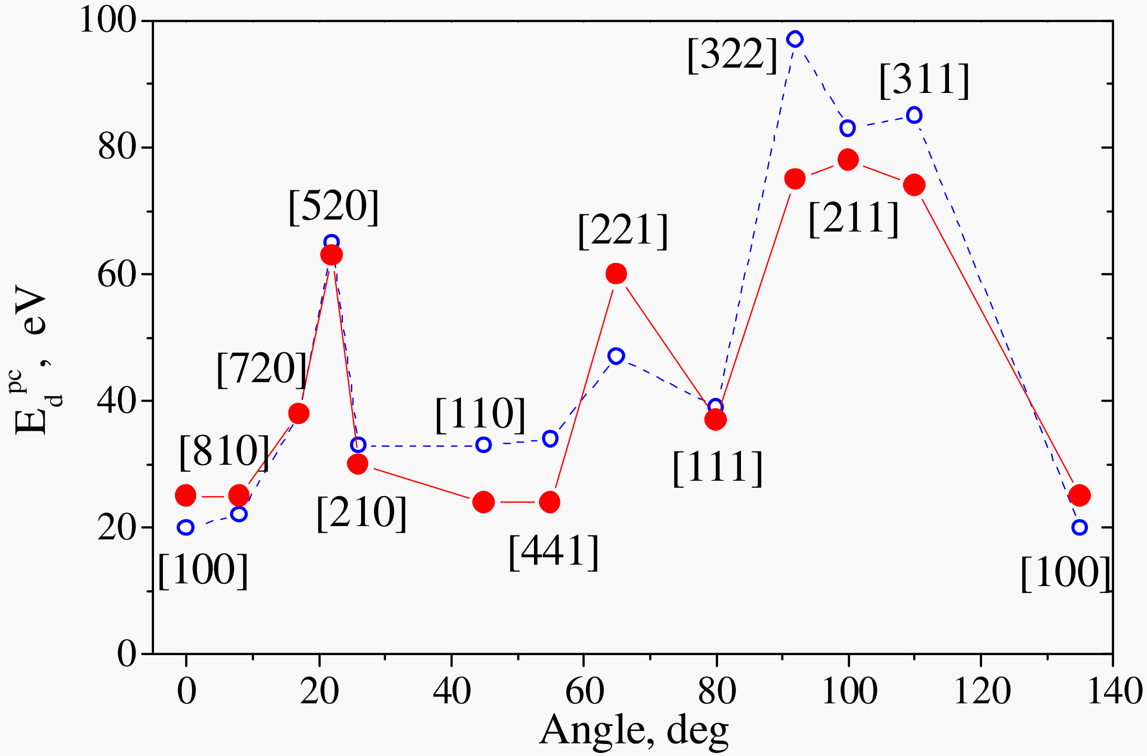
The initial sizes of voids are varied from 312 to 1004 atomic volumes. PKAs are generated at about 3-5 atomic distances from the void.



The collision events close to voids results in a biased formation of vacancies due to the lower energy barrier involved

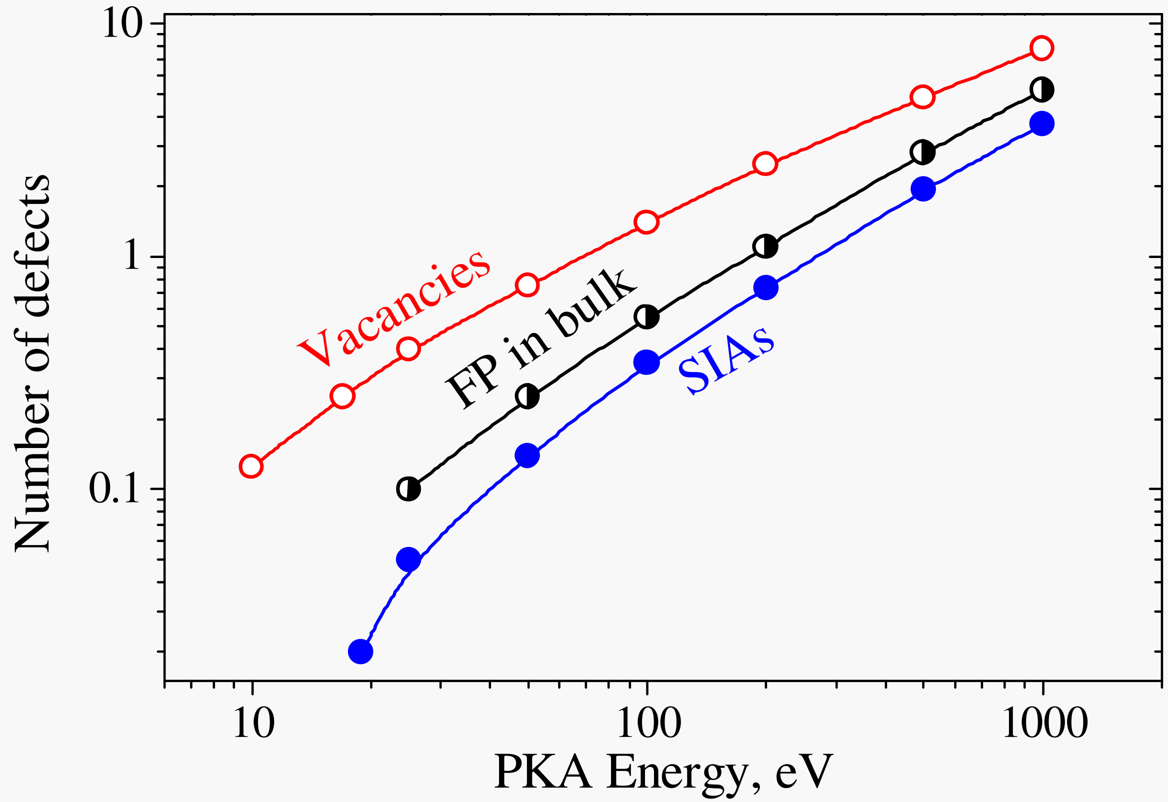
Displacement threshold energy in bulk Cu at T = 4 K

N. P. Lazarev, V. I. Dubinko, Radiat. Eff. & Def. Solids 158 (2003) 803.
D. J. Bacon, H. F. Deng, F. Gao, J. Nucl. Mater. 205 (1993) 84.



The lowest threshold energy is about 25 eV. PKA in the direction close to <110> generates replacement collision sequence and produce stable Frenkel defects separated by large distances starting from l = 4 at 24 eV to tens inter-atomic distances at higher energies.

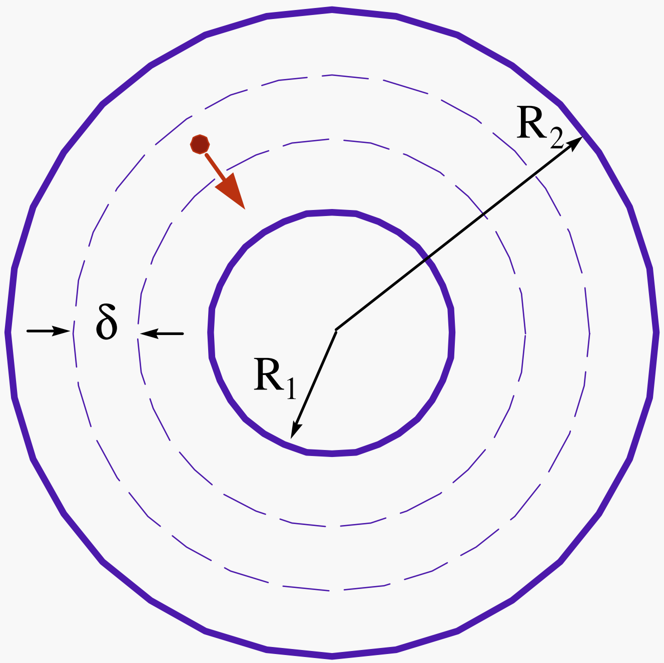
A biased formation of vacancies in the vicinity of void



The ratio N_v / N_i amounts to about 8 at 25 eV and decreases to ~2 at 1 keV.

The effect decreases with increasing distance from the void surface.

Simulation of void dissolution by subthreshold irradiation



Schematic picture of void inside solid sphere. PKA ranges in between of two spheres depicted by dotted lines.

Initial sizes: R_1 = 15 Å, and R_2 = 45 Å. N = 31872 atoms.

Every about 35 ps a new collision with E_K = 18 eV was generated.

Time of thermal dissolution of void

$$dV/dt = 4\pi D_v R\left(\overline{C}_v - C_v^b\right) \qquad C_v^b = C_v^0 \exp\left(2\gamma/R\right) \qquad \gamma = \sigma\omega / kT$$

$$dR/dt = \left(1 - \exp(2\gamma/R)\right) D_v C_v^0 / R$$

$$\tau_{th} = \frac{R_0^3}{2\gamma D_v C_v^0 \left(2 + \exp(2\gamma/R_0)\right)}$$

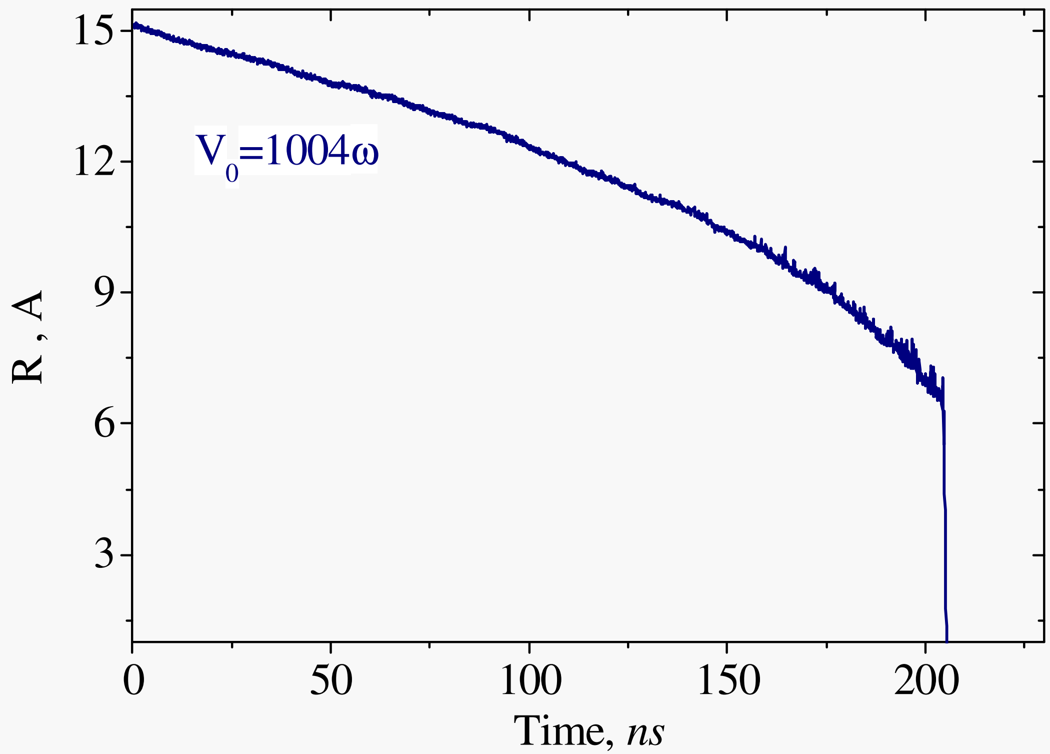
At T = 1000 K, R_0 = 15 Å, energetic parameters of Cu, the estimated time τ_{th} is about 0.3 *ms* which is far above the time accessible in usual MD simulations

Time dependence of void size during irradiation

$T = 1000$ K

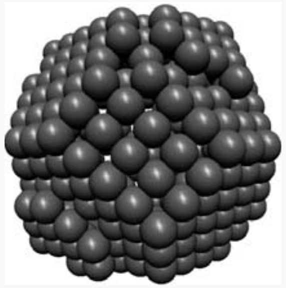
$E_K = 18$ eV

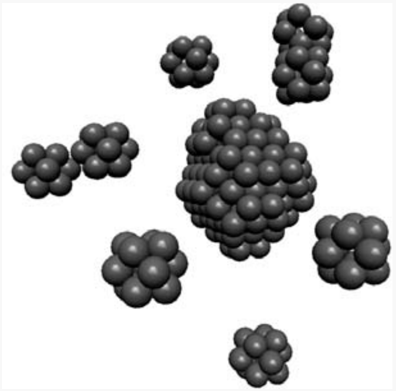
>5000 cascades

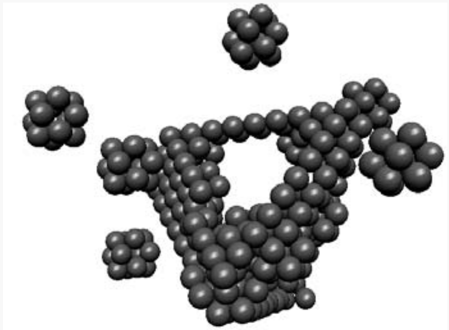


The void has been dissolved completely: at R = 6 Å, the void has been transformed to a stacking fault tetrahedron.

Different stages of void dissolution


Initial void


Dissolved void after ~200 ns


Beginning of SFT formation

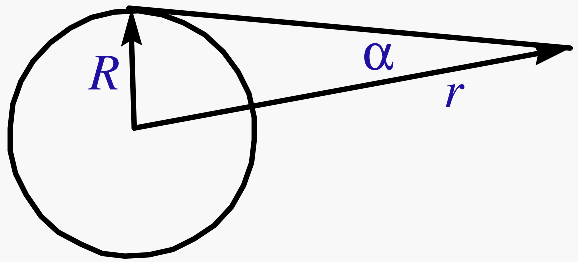

Final state of SFT development

Void dissolution rate due to radiation emission of vacancies

Only PKAs directed towards the void create vacancies.

Vacancy generation rate:

$$K^*(r,R) = \frac{K(r,R)}{2}\left[1-\sqrt{1-\frac{R^2}{r^2}}\right]$$



$$K(r,R) = \begin{cases} K_0, & R < r < R+\Delta \\ 0, & otherwise \end{cases}$$

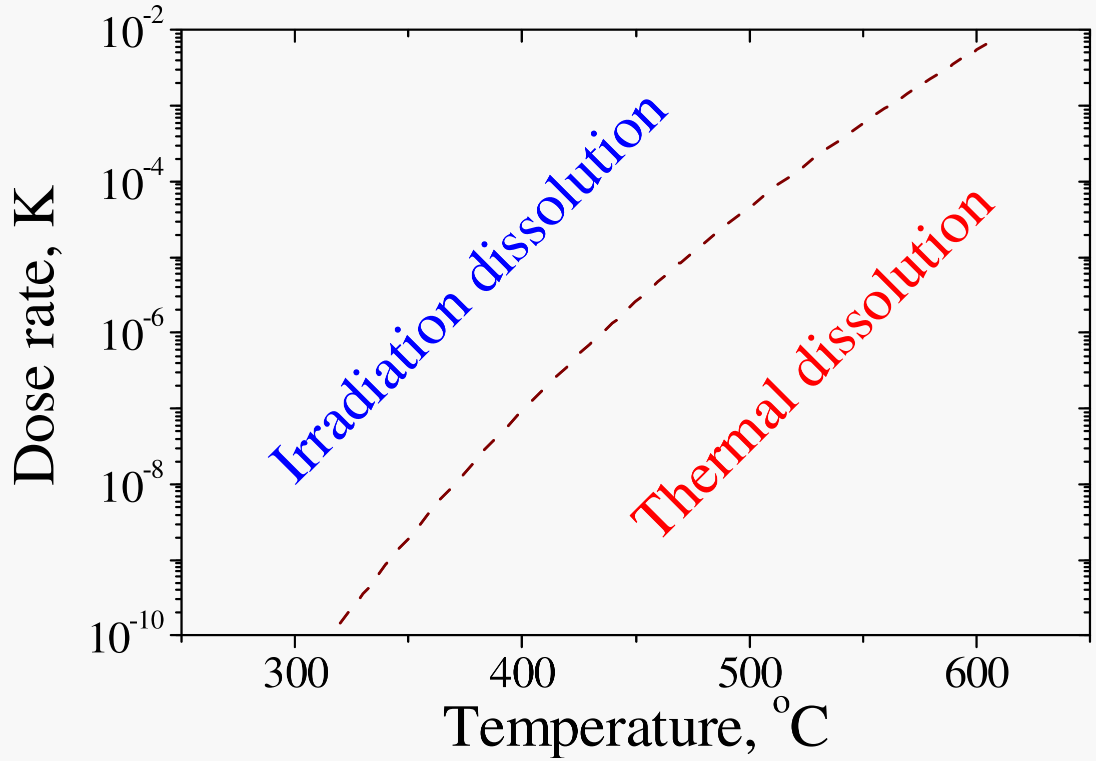
Fluxes of the radiation-emitting and thermal vacancies:

$$J_v^{irr} \approx \pi K_0 \frac{R^2\Delta^2}{R+\Delta} \qquad J_v^{th} = 4\pi R D_v C_v^0 \exp(2\gamma / R) \qquad \gamma = \sigma\omega / kT$$

Effective vacancy concentration at void under irradiation:

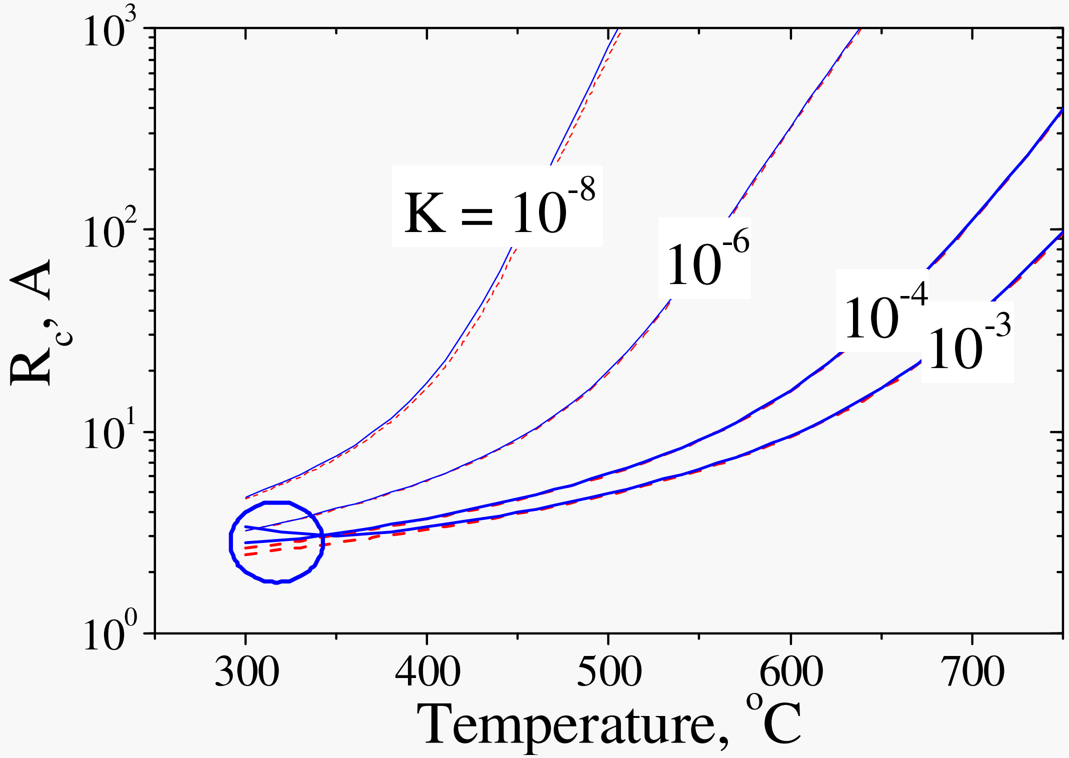
$$C_v^b \to \tilde{C}_v^b = C_v^0 \exp(2\gamma / R) + \frac{R\Delta^2 K_0}{4D_v(R+\Delta)}$$

Void dissolution rate due to radiation or thermal vacancies



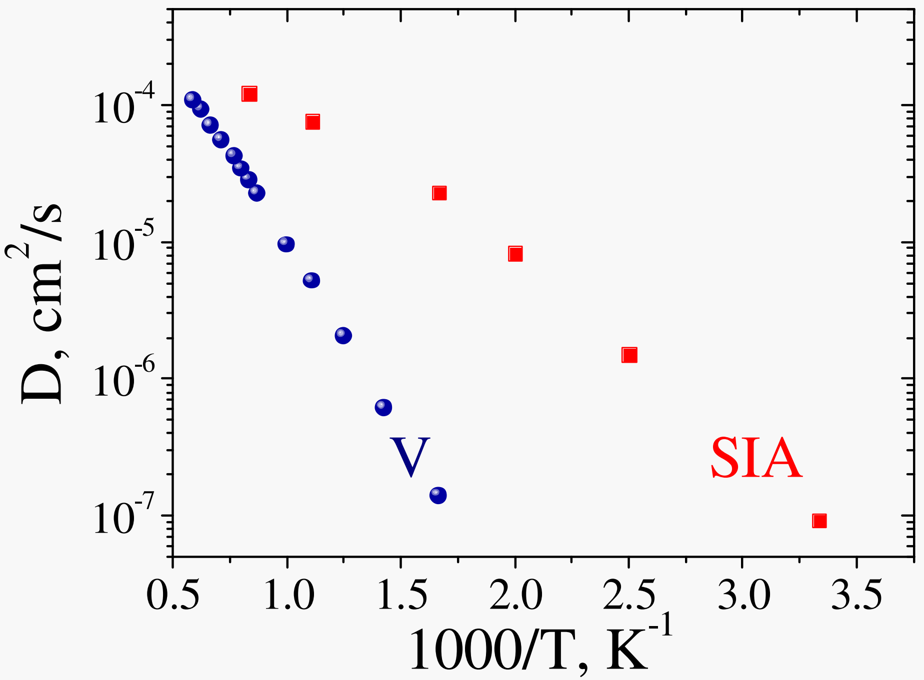
The rate of radiation-induced void shrinkage is proportional to the dose rate K_0 and it is expected to increase with increasing range of focusing collisions as irradiation temperature decreases.

Critical size of a void *vs* temperature and dose rate



Radiation dissolution appreciably increase the critical size only at low temperatures and high dose rates.

Diffusion and primary damages in Fe



Migration energy of vacancy diffusion $E_v^m = 0.58$ *eV*

and of SIA diffusion $E_i^m = 0.28$ *eV*

The size of simulated box L has to be much larger than diffusion range: $L^2 >> 6D_i t_s$ *, where* $t_s \sim 100$ *ps*

Primary damages in displacement cascades

$N = 10^5 - 2{\cdot}10^6$

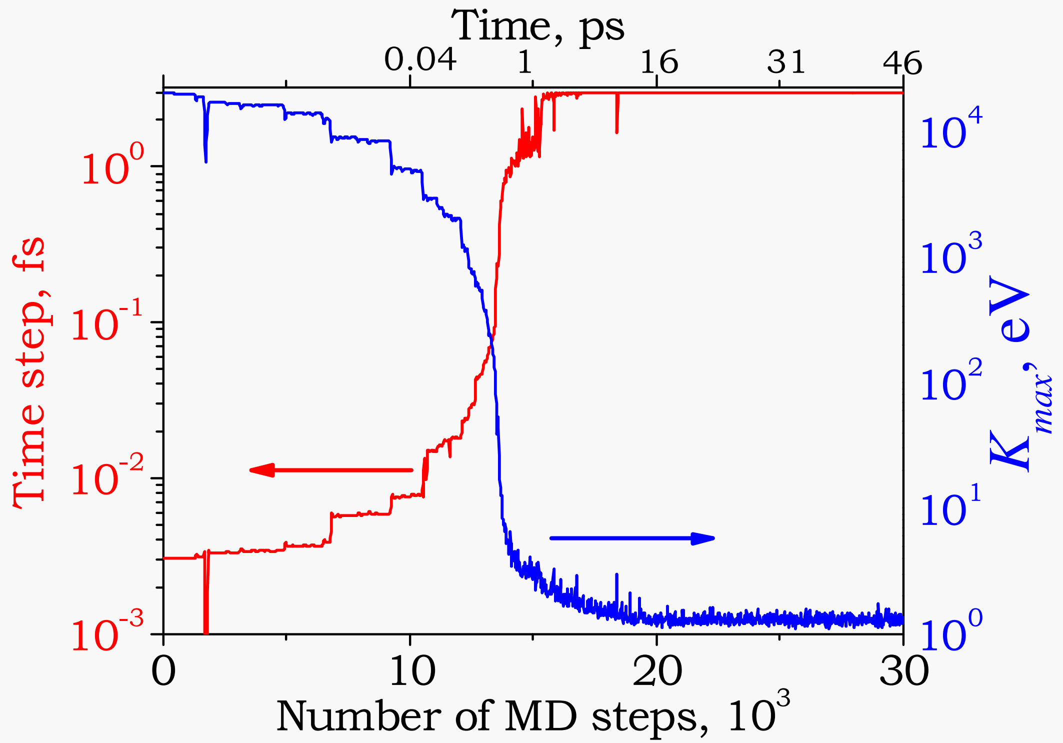
PKA energies: 0.01 – 20 keV

Temperatures: 300, 600, 900 K

Cascades at every point (E_d, T): > 50

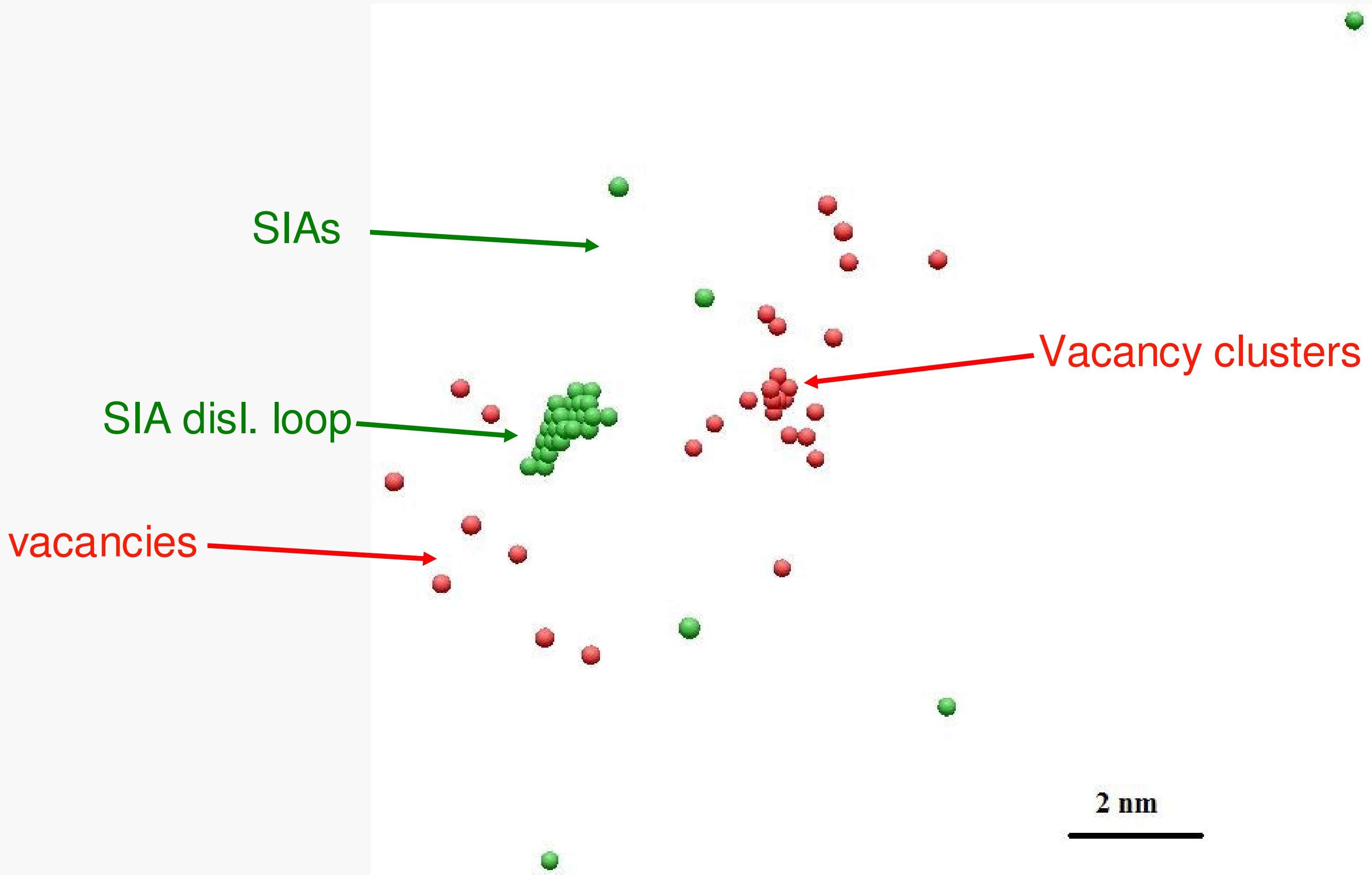
Total number of cascades: > 5000

Variable time step. E_{PKA} = 20 keV, T = 900 K



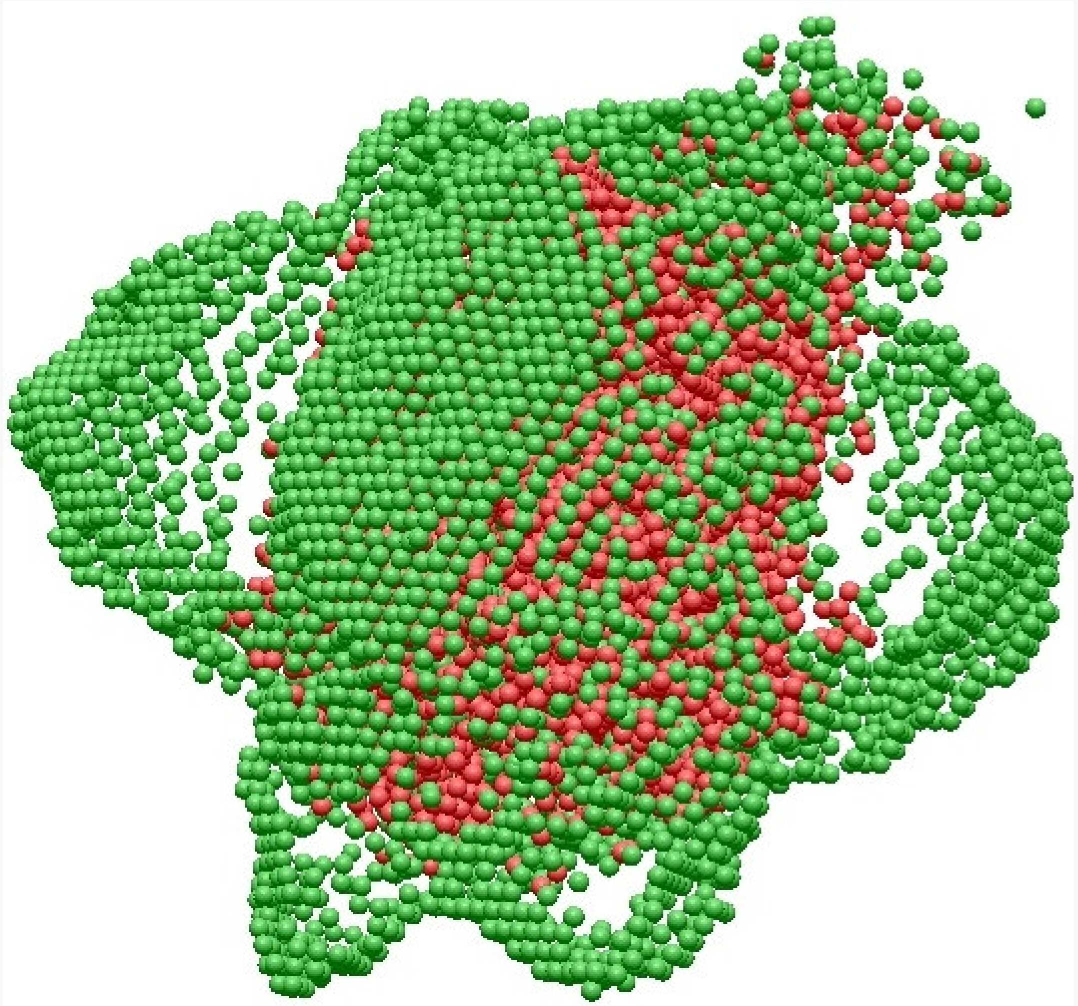
A typical evolution of the time step and energy of fastest atom.
Ballistic stage of cascade development runs out in about 1 ps.

Point defect distribution, E_{PKA} = 20 keV, T = 900 K



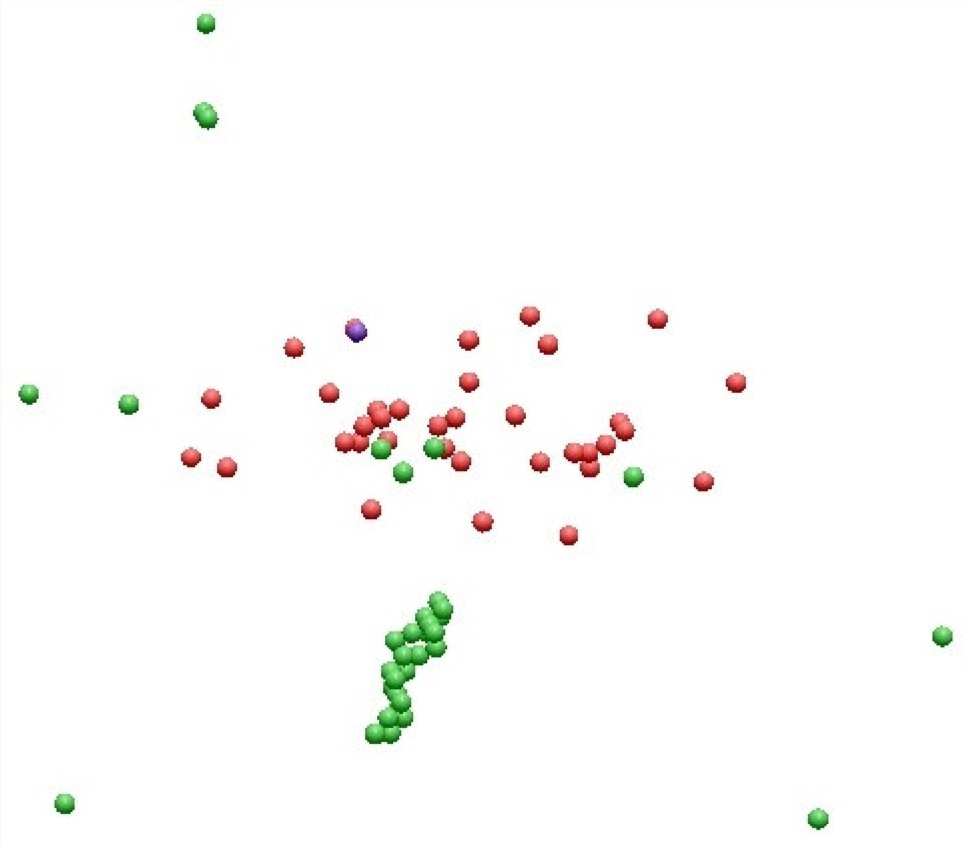
Cascade evolution in time. 1 frame per 500 MD time steps

E_{PKA} = 20 keV,
T = 900 K

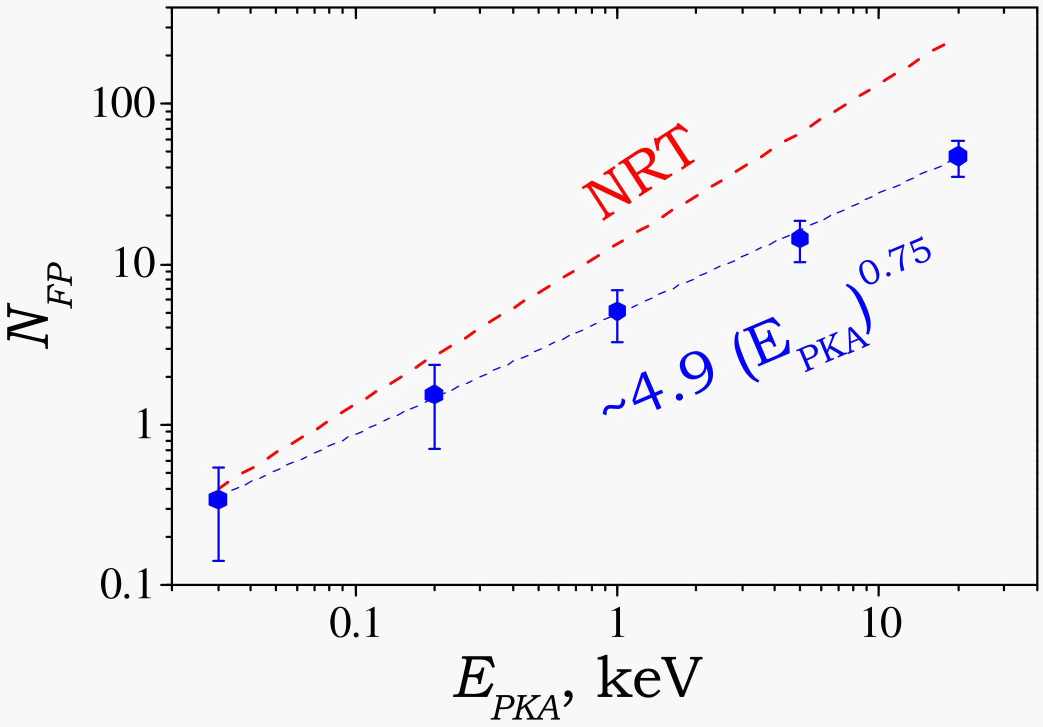


Cascade evolution in time, another view

E_{PKA} = 20 keV,
T = 900 K



Defect production in perfect crystal at T = 300K

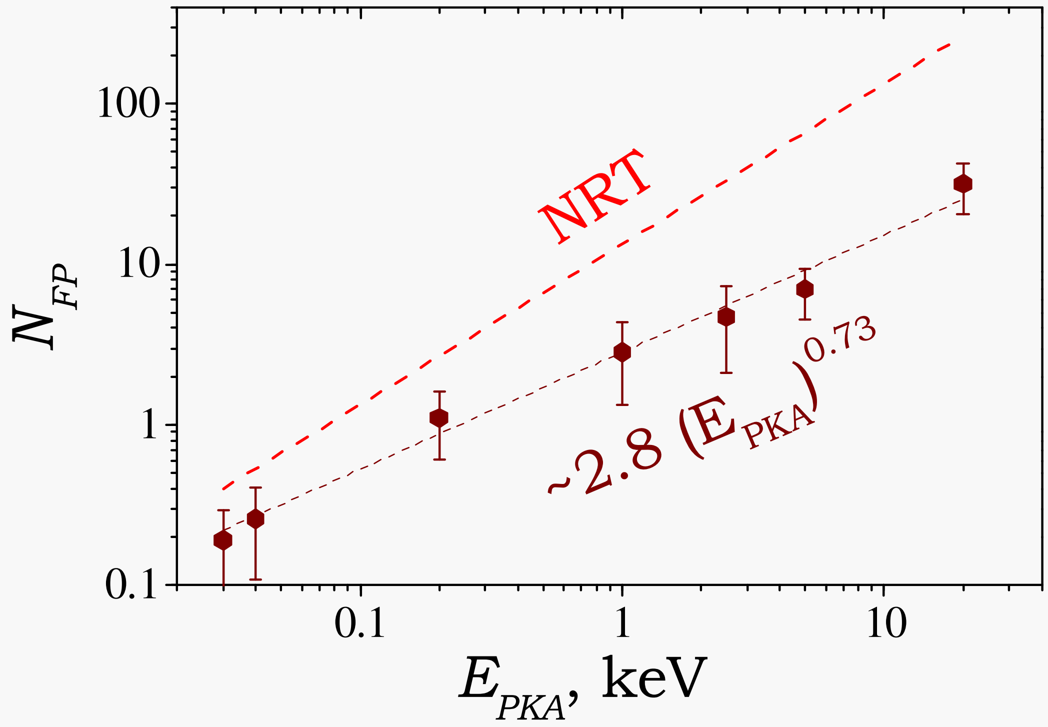


The standard Norgett-Robinson-Torrens (NRT) theory:

$$N_{NRT} = 0.8\ E_D\ /2E_d$$

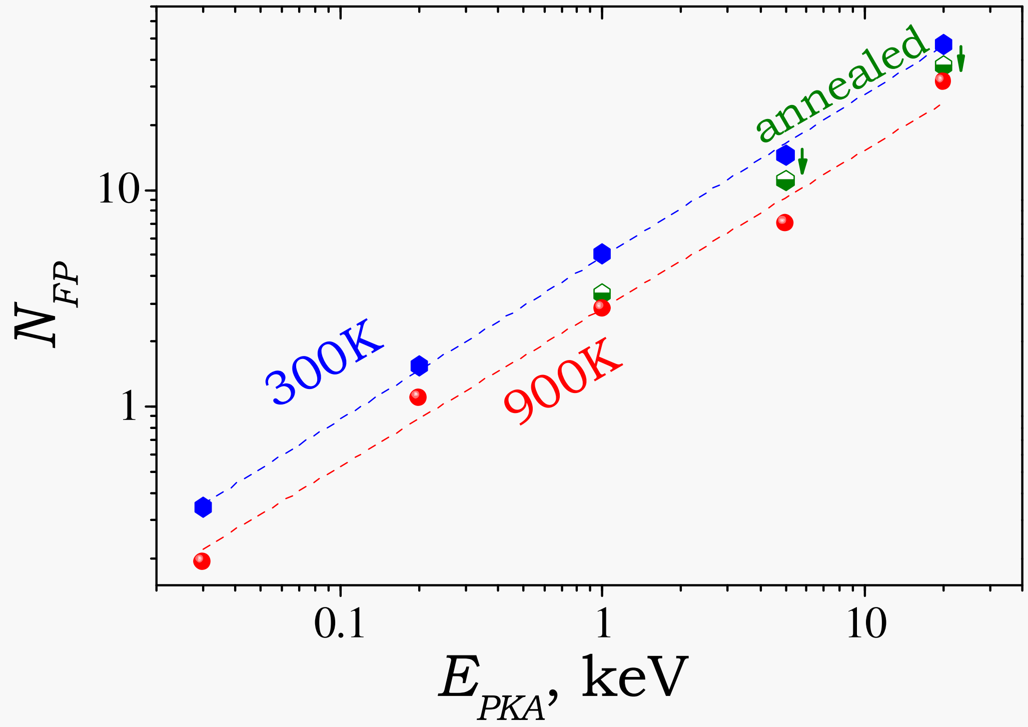
For simulated Fe we estimate threshold energy $E_d = 30$ *eV*

Number of Frenkel pairs vs. PKA energy at T = 900K



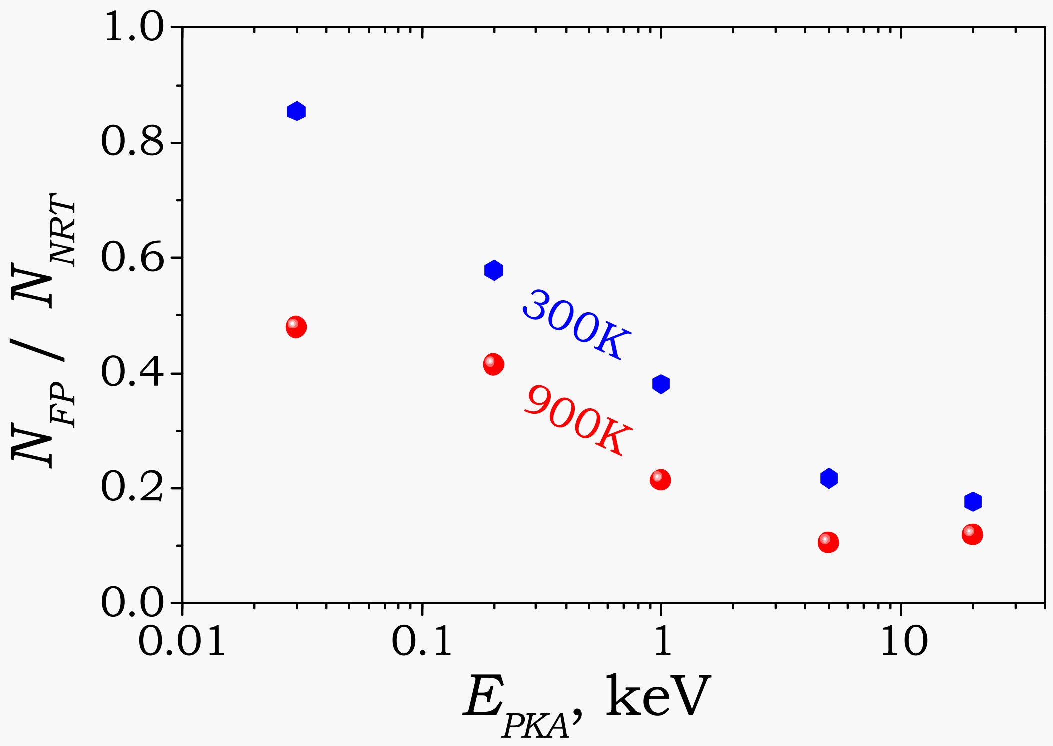
The number of the survived point defects decreases when the temperature rises. One can expect the reduction of the effective volume of a cascade and the increase of the lifetime of the thermal spike at high temperature. Both factors enhance the recombination of defects.

Effect of cascade defects annealing at high temperature



Annealing of low temperature cascade defects smoothes over the temperature effect

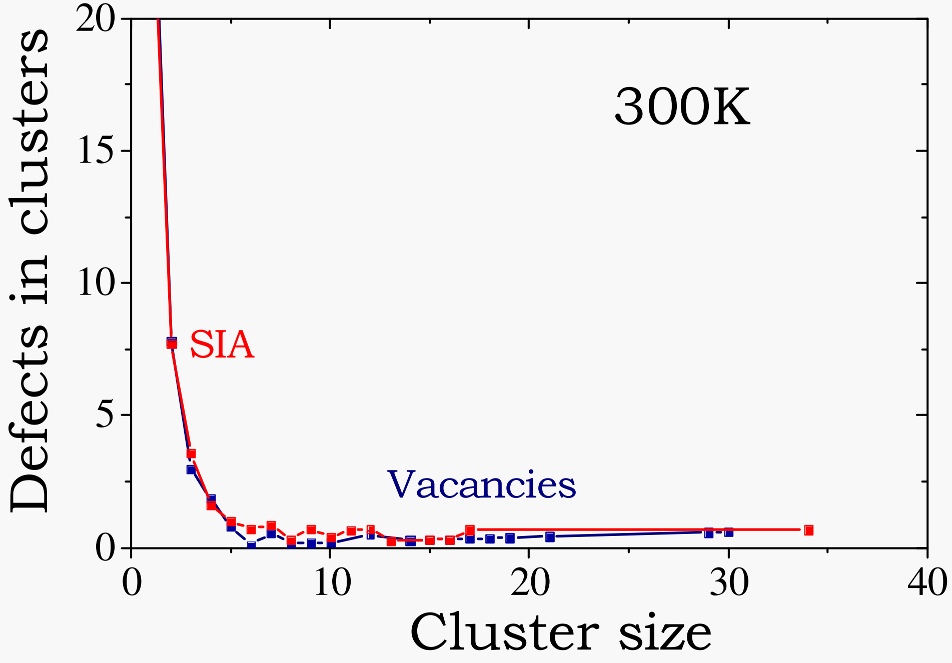
Survived point defects fraction

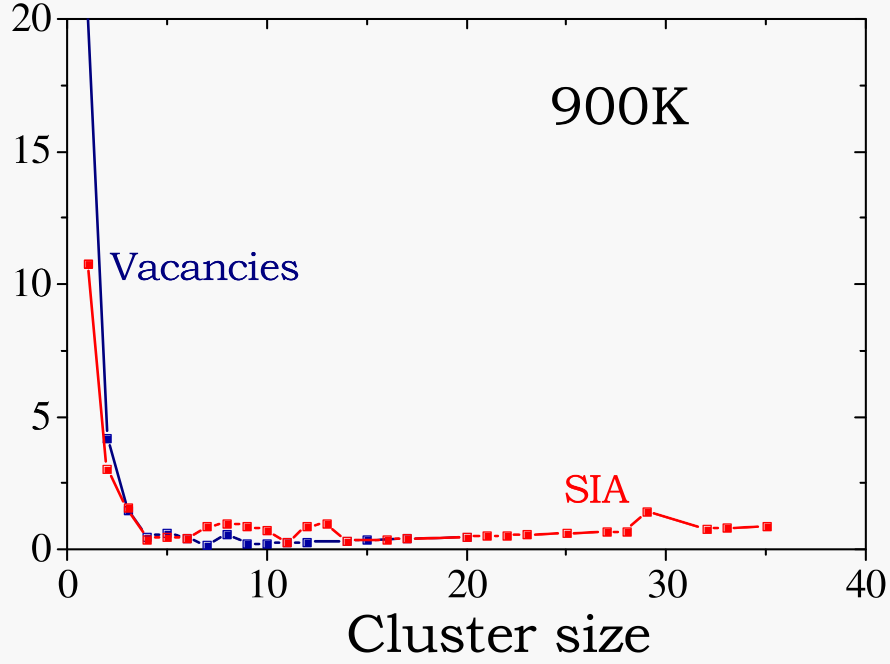


Damage production efficiency is degraded with increase of cascade energy

Distribution of cluster sizes

20 keV





Both vacancies and especially SIAs tend to aggregation with the growth of temperature

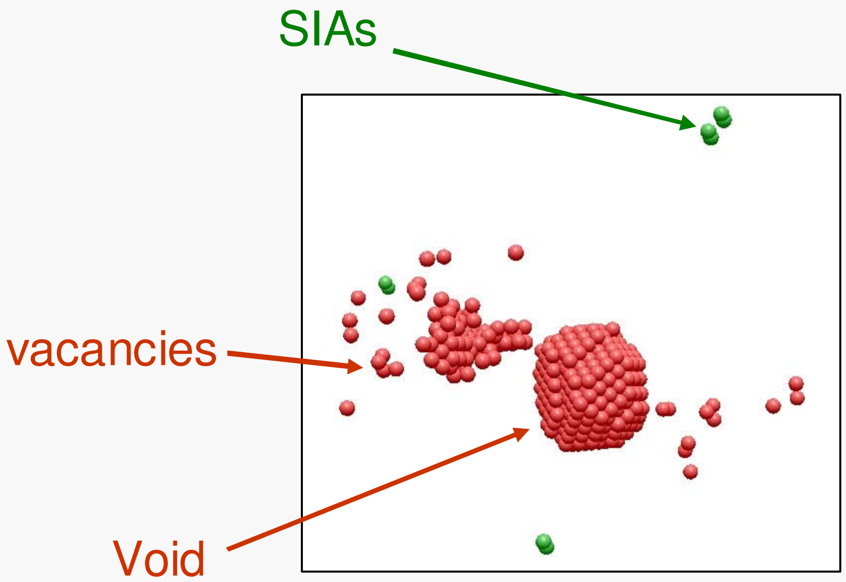
Defects production near voids

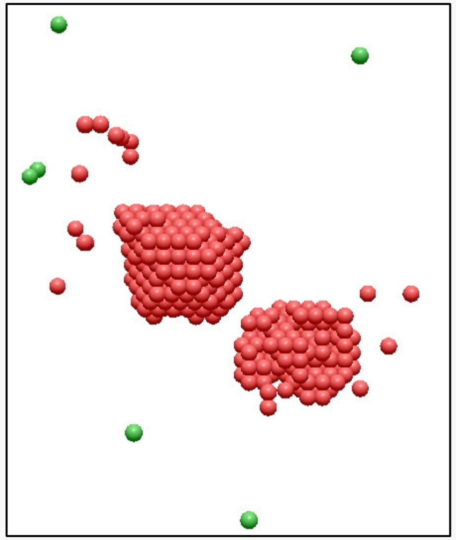
$N = 10^5 – 2 \cdot 10^6$

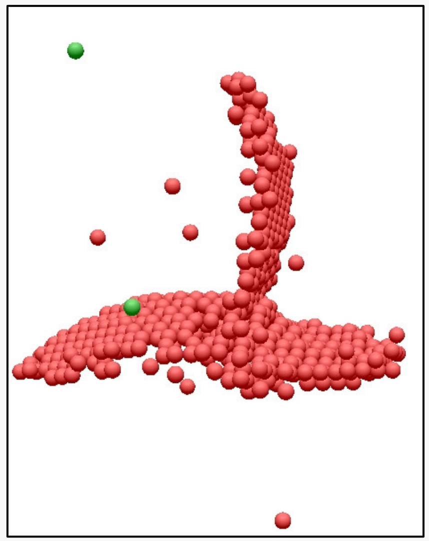
PKA energies: 1 – 20 keV

Sizes of voids: 312 - 1004 v_a

Some final states of cascade development near voids



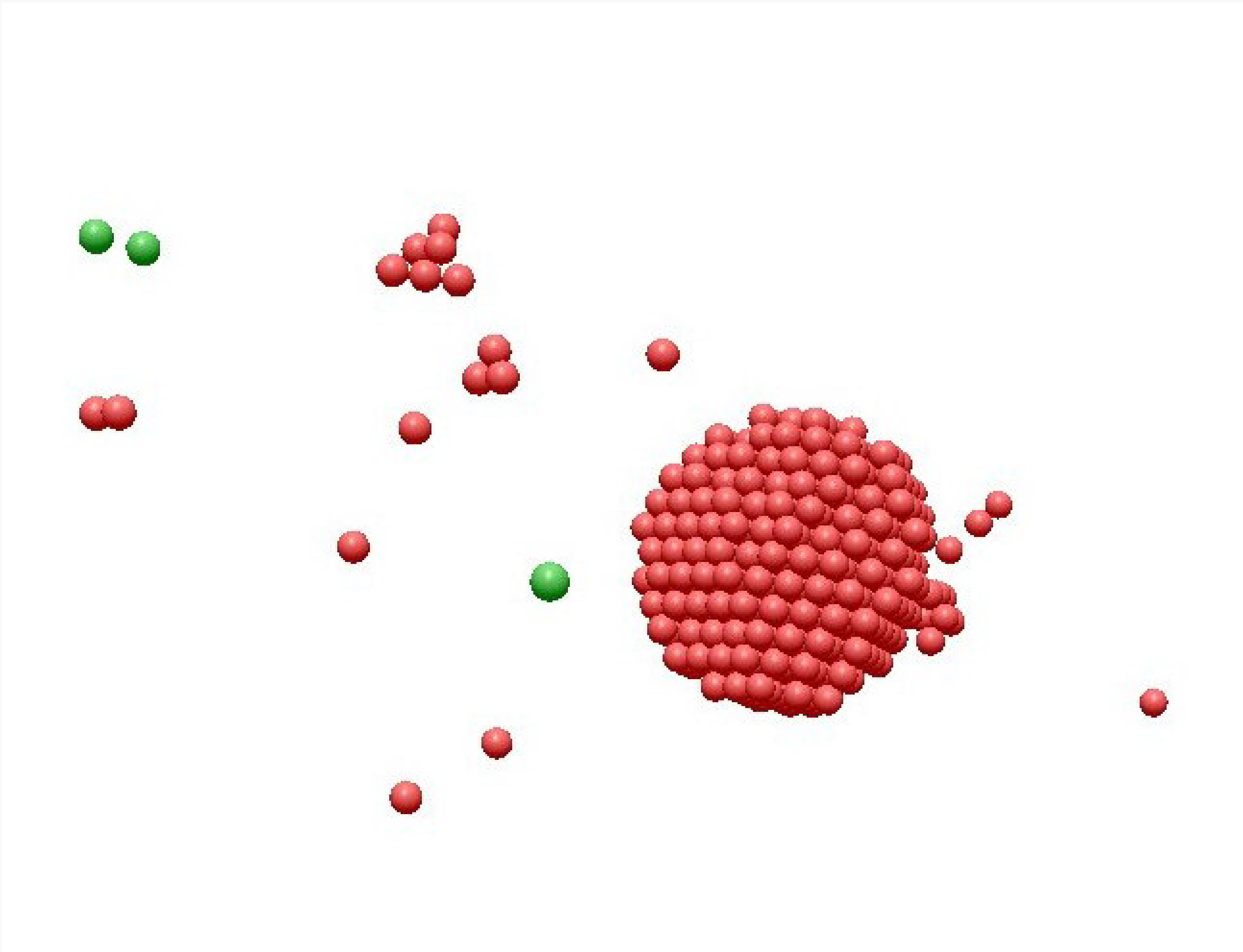




E_{PKA} = 8 keV, T = 900 K

Cascade evolution near a void. 1 frame per 500 MD time steps

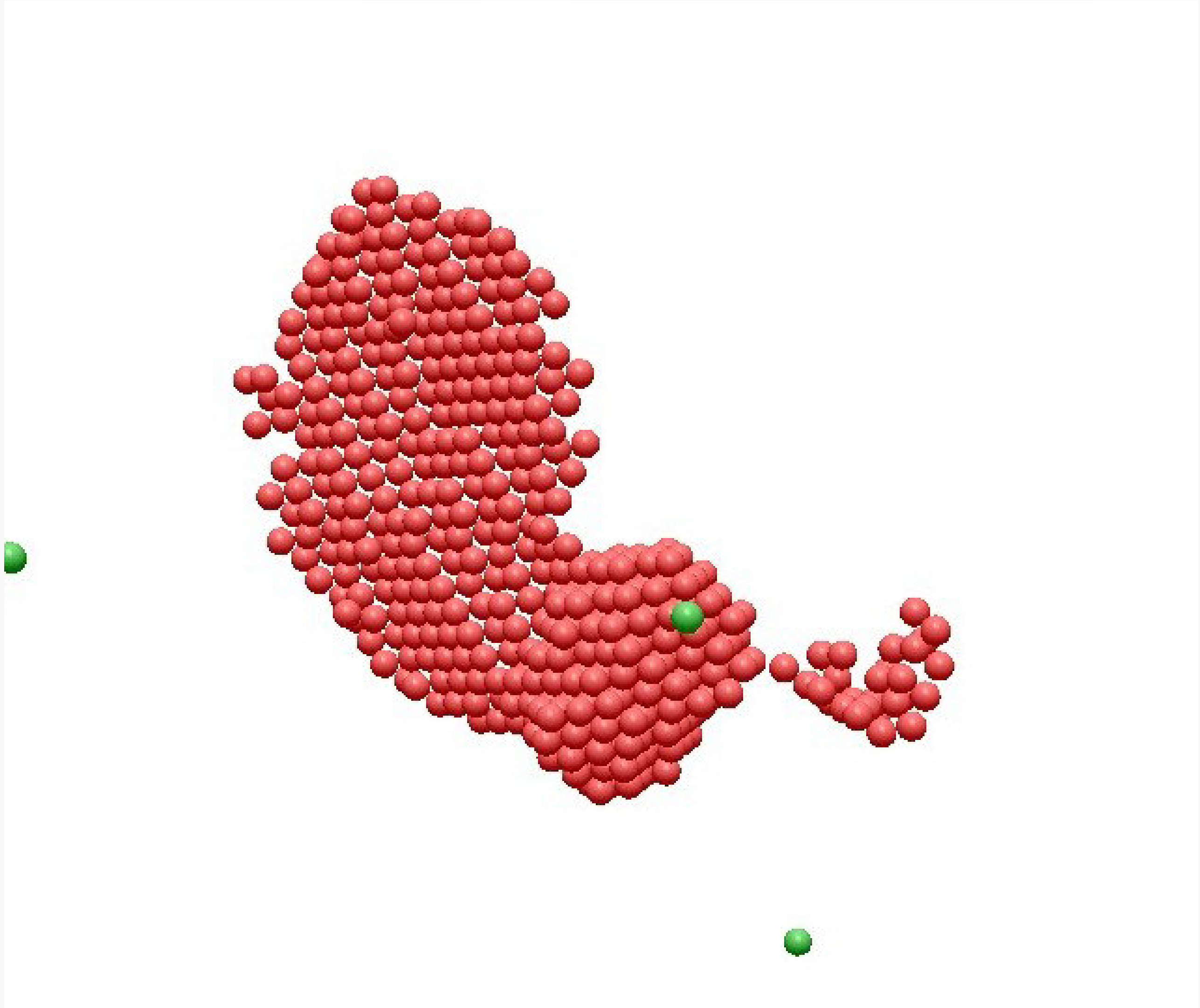
E_{PKA} = 8 keV, T = 900 K



Cascade evolution near void. 1 frame per 500 MD time steps

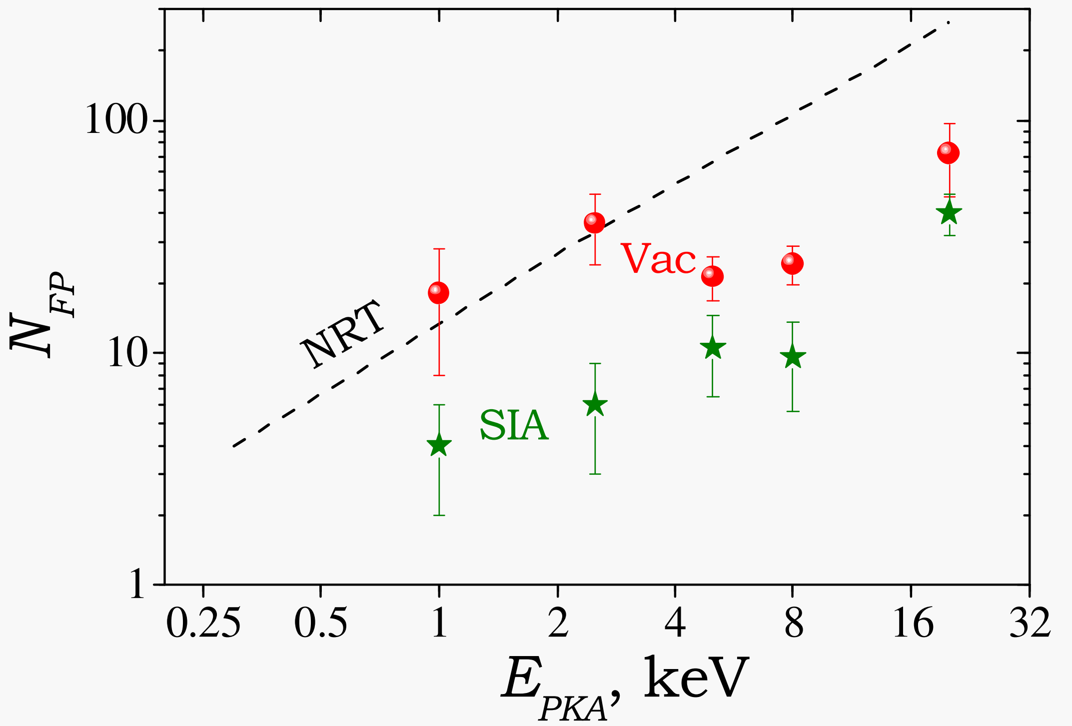
E_{PKA} = 8 keV

T = 600 K



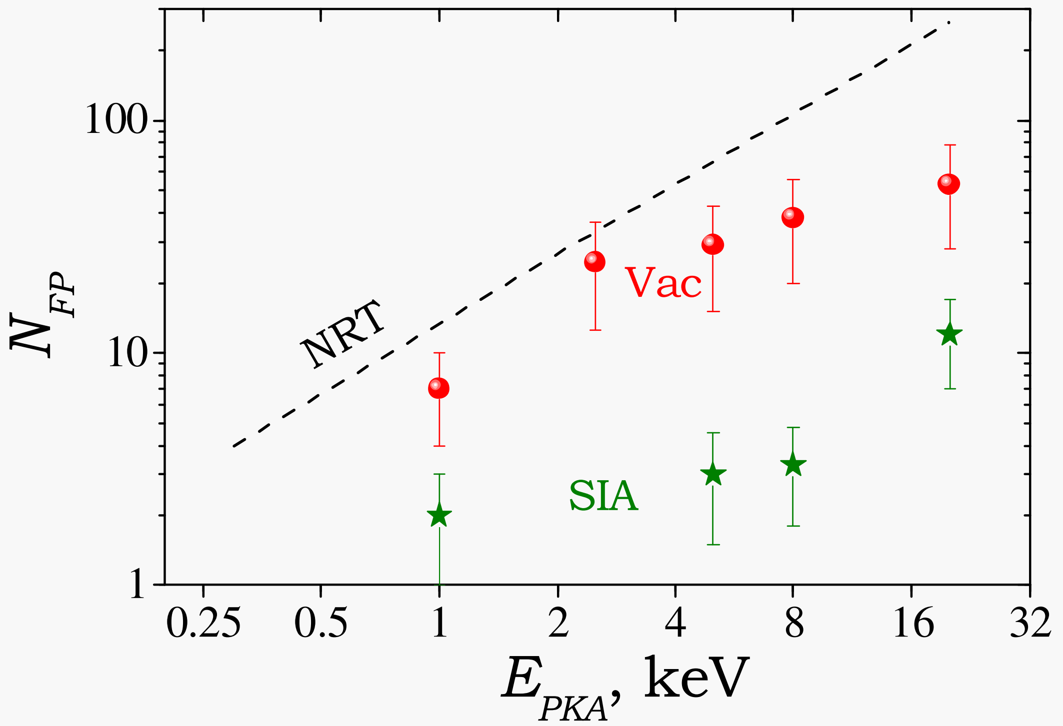
Destroying of void by nearby cascade

Defect production near voids at T = 300K



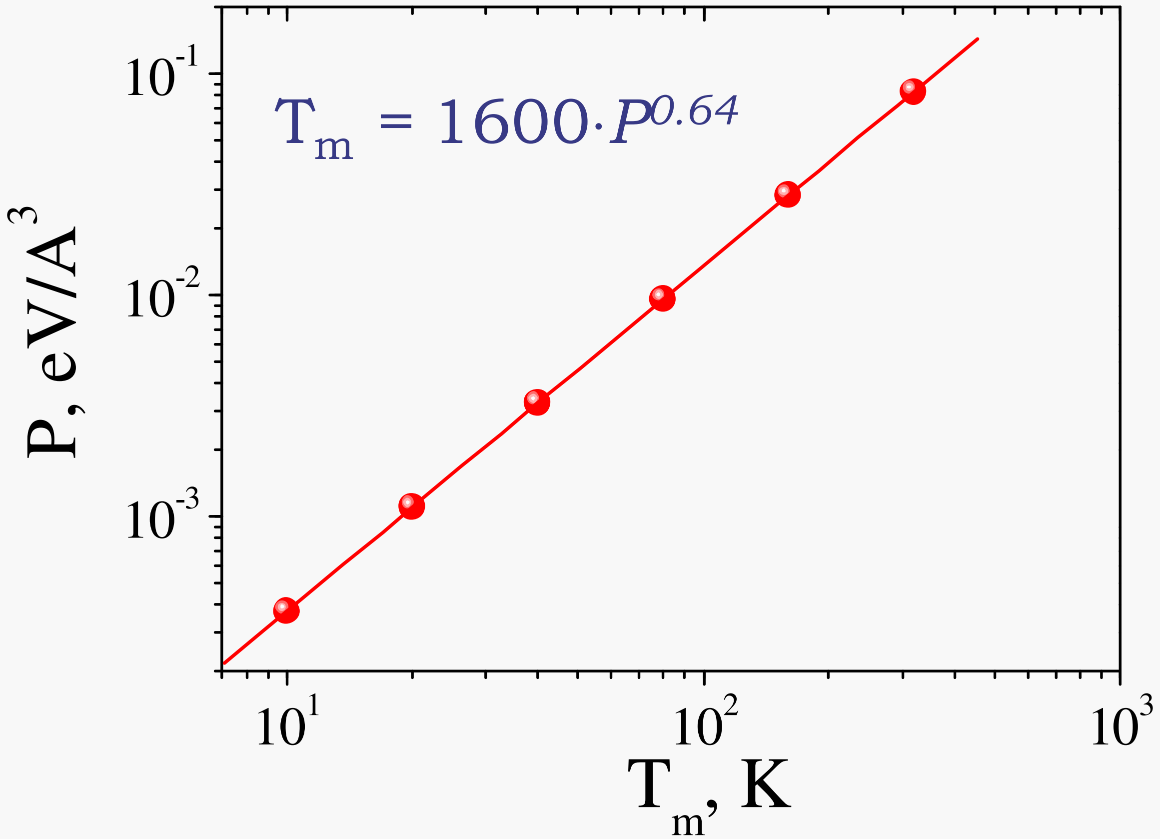
Biased creation of vacancies compared to interstitials is observed for all studied energies

Defect production near voids at T = 900K



Effect of preferential creation of vacancies is enhanced at high temperature

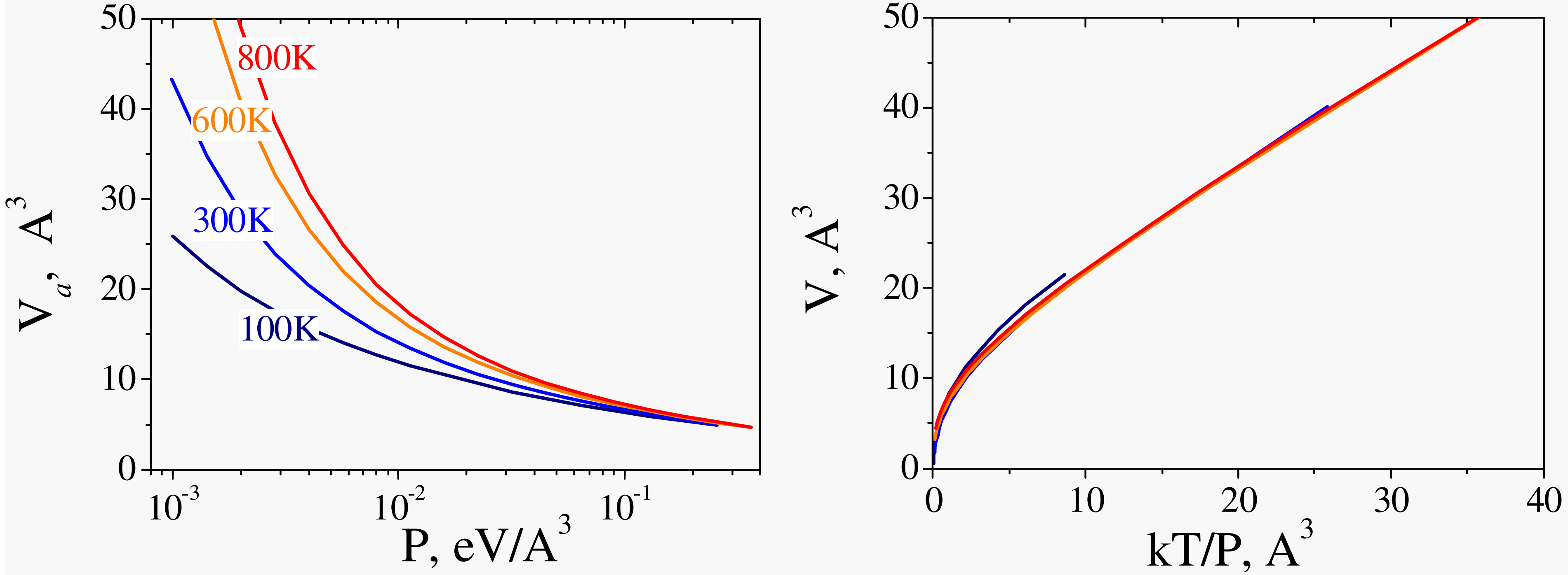
Melting temperature of He *vs* pressure



The melting temperature is found by studying the equilibrium of coexistence of liquid and crystalline phases.

At P = 0.1 eV/Å³ = 16 GPa, the T_m *> 300 K and it should be expected that helium can be found in bubbles exactly in solid state. Even at high temperature the helium in the bubbles is in a liquid state.*

Equation of state for Helium



$$PV/kT = f(V)$$

Balescu R., Equilibrium and non-equilibrium statistical mechanics, 1975

Defects production near He bubbles

$N = 10^5 – 2{\cdot}10^6$

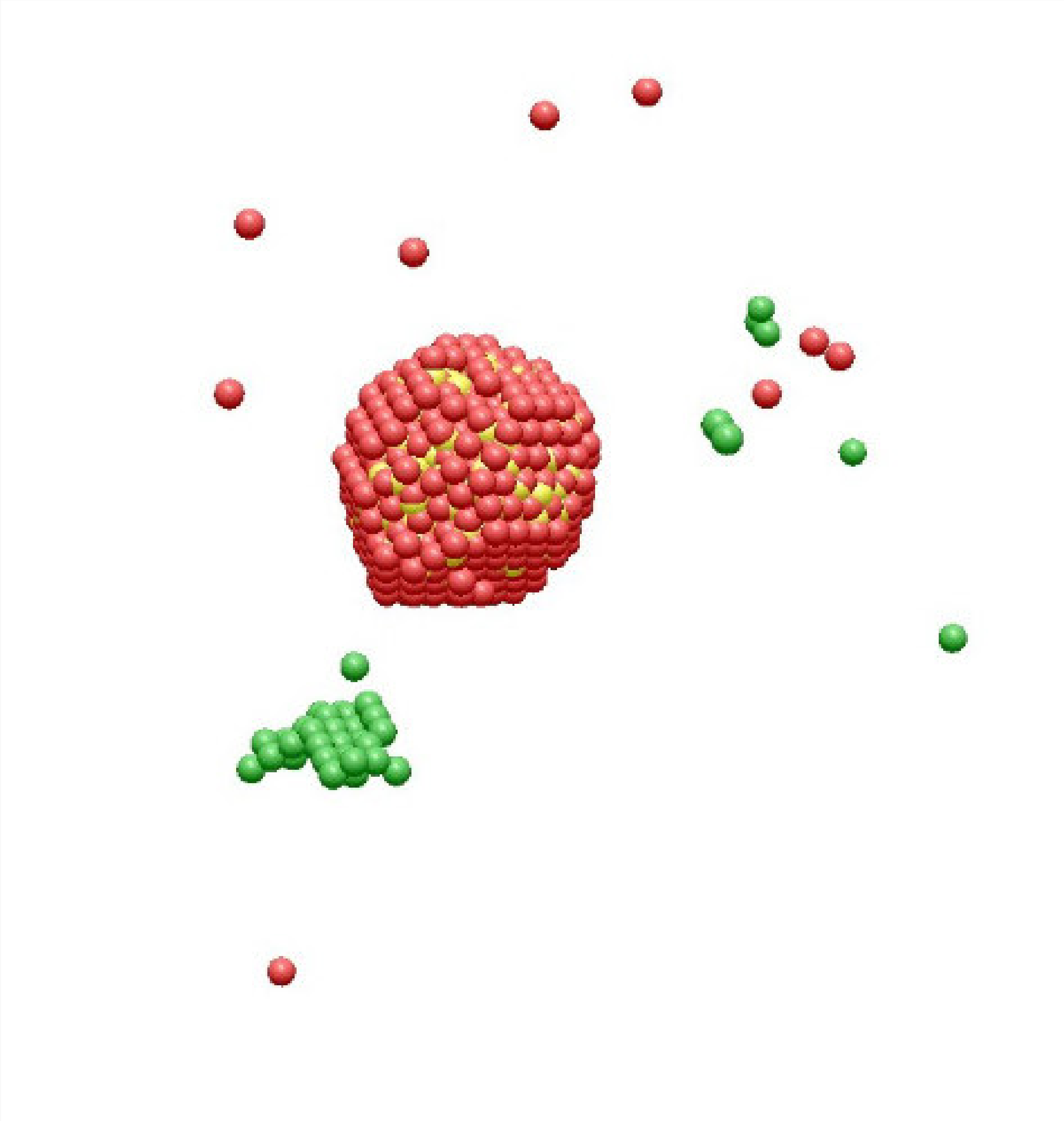
PKA energies: 1 – 20 keV

Sizes of bubbles: 312 v_a

He/V = 1

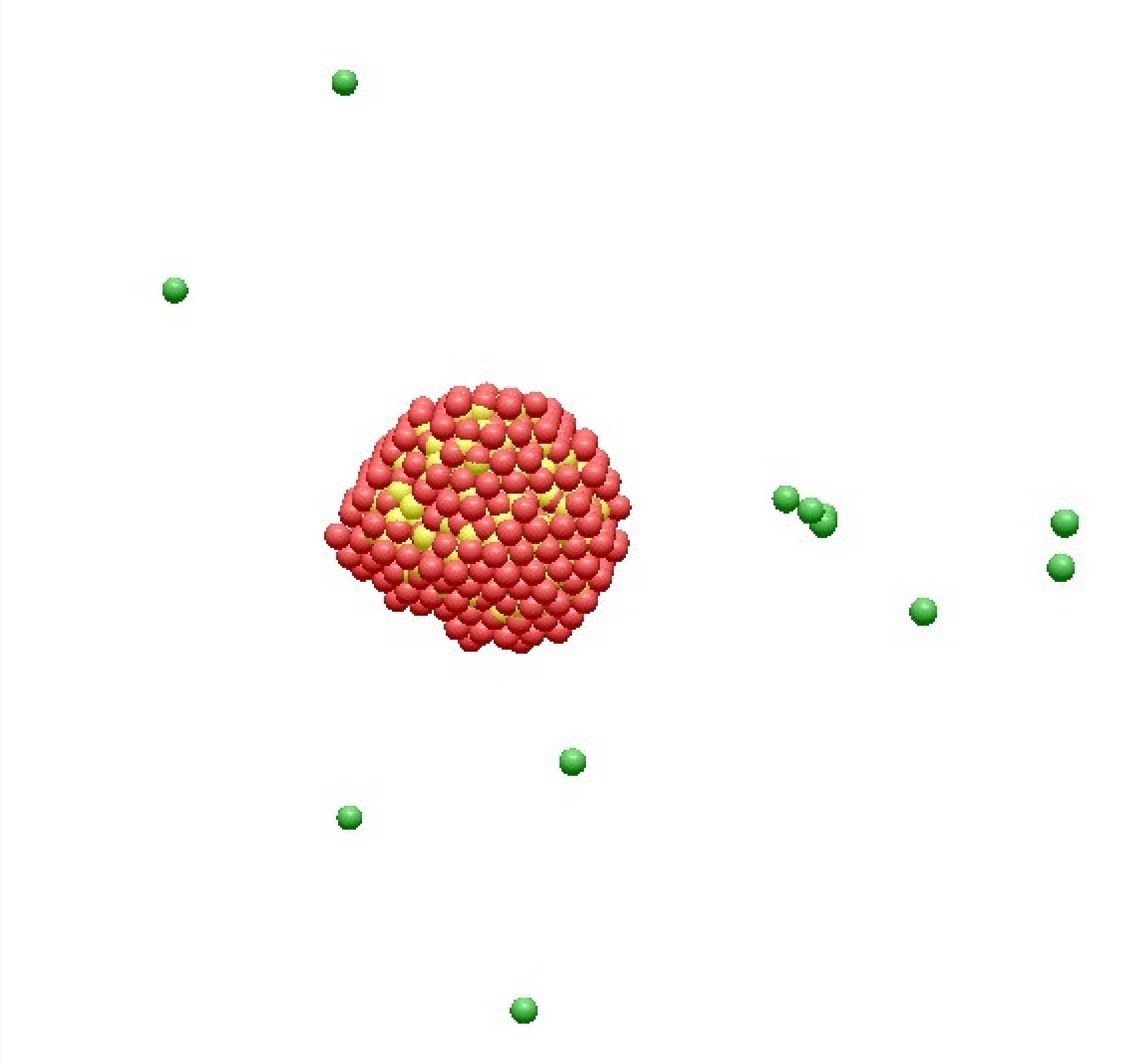
Cascade evolution near bubble. 1 frame per 500 MD time steps

E_{PKA} = 8 keV
T = 900 K

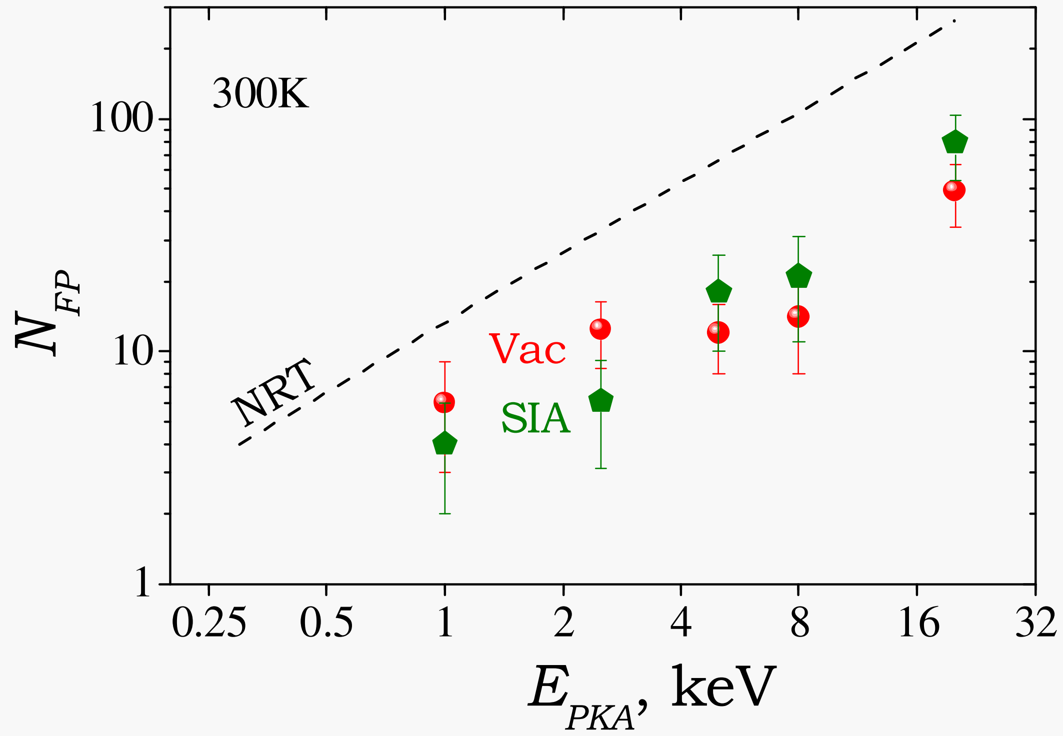


Cascade evolution near bubble. 2-nd example

E_{PKA} = 8 keV,
T = 900 K

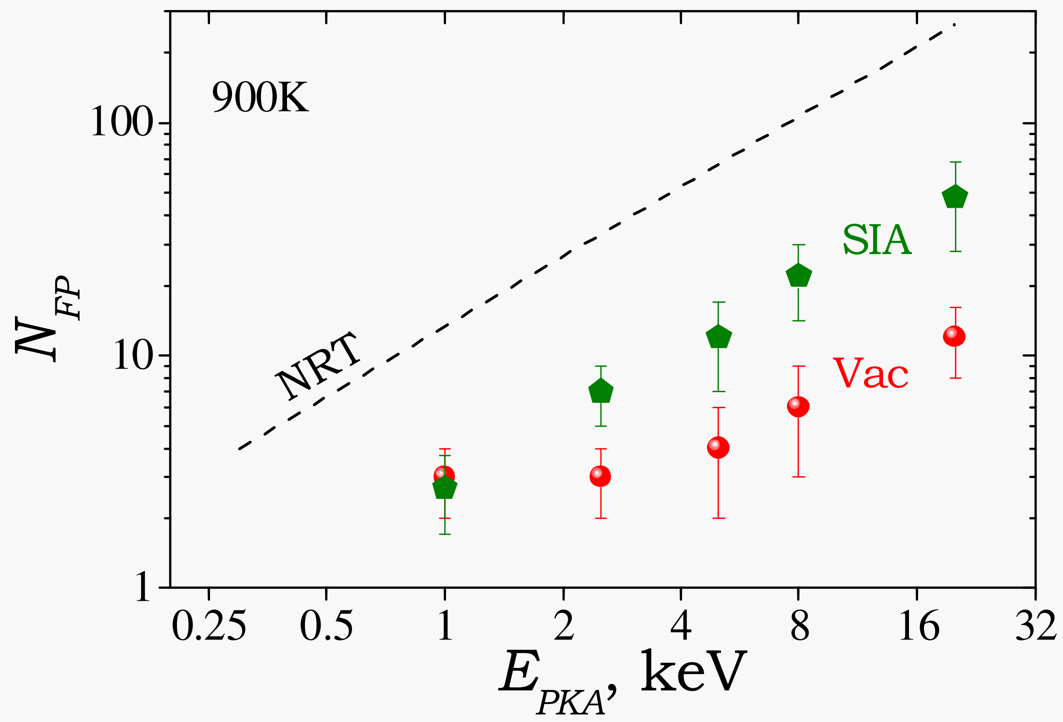


Defect production near bubbles at T = 300K



Biased creation of vacancies at low E_{PKA} and SIAs at high PKA energy

Defect production near bubbles at T = 900K



Biased creation of SIAs at all PKA energies

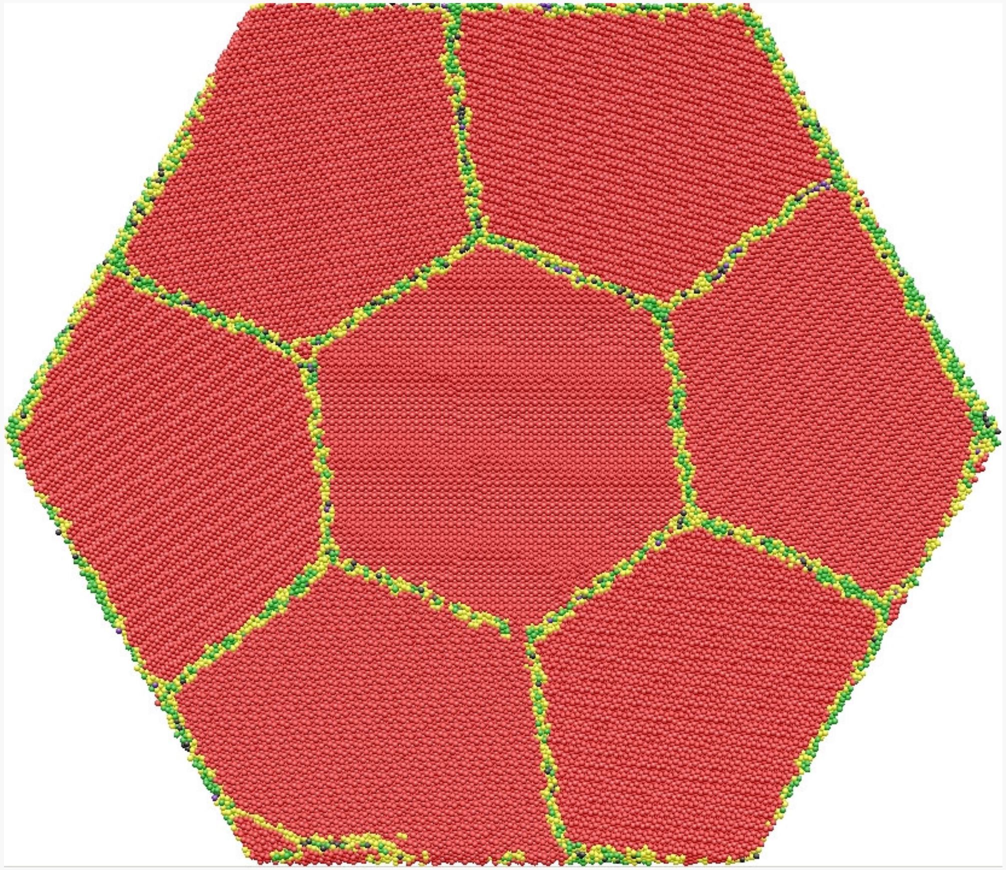
Simulation of recrystallization under irradiation

The polycrystal prepared by Voronoy method.

Number of grains is 13.

Total number of atoms is 3201384.

Mean size of the grain is 15 nm.



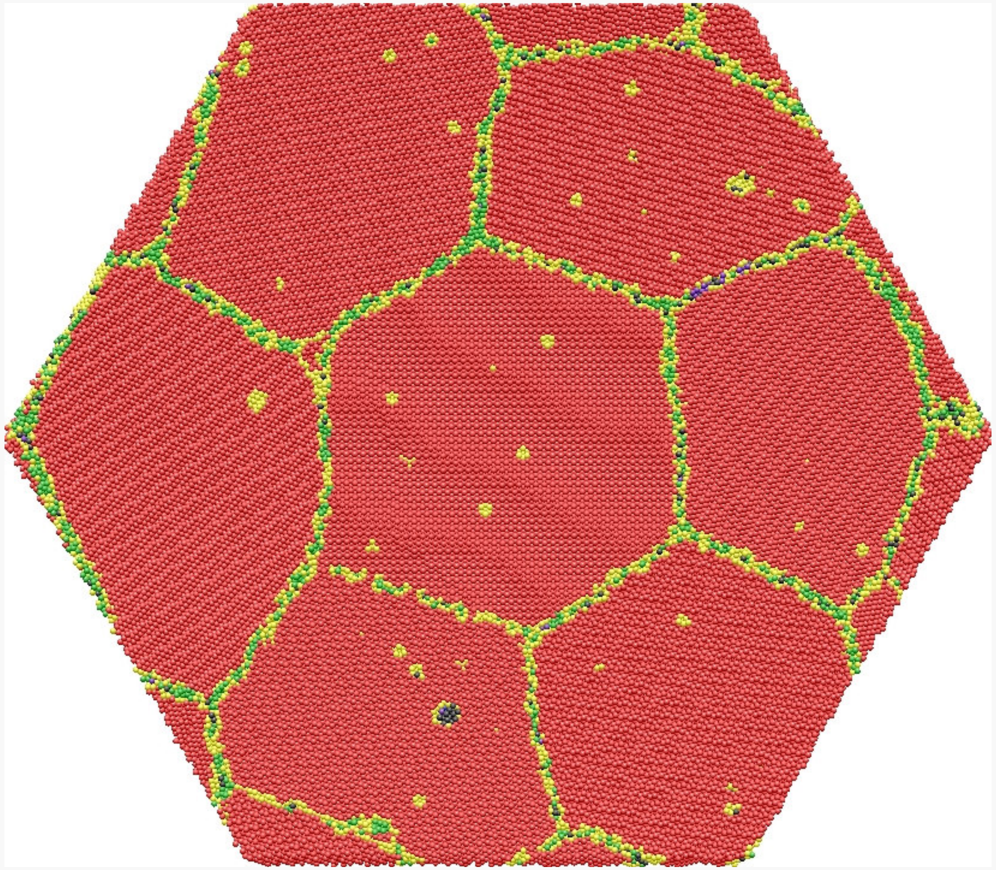
The initial state after the high-temperature annealing. The cut of the polycrystal is taken in the central part of the cubic specimen.

Homogeneous irradiation of polycrystal

A cascades with the energy 5 keV were generated every 8 ps.

The effective irradiation dose can be estimated as 10^{-2} dpa.

The most part of created defects are vacancies and vacancy clusters (voids).



The polycrystal state after homogeneous irradiation by 800 cascades with

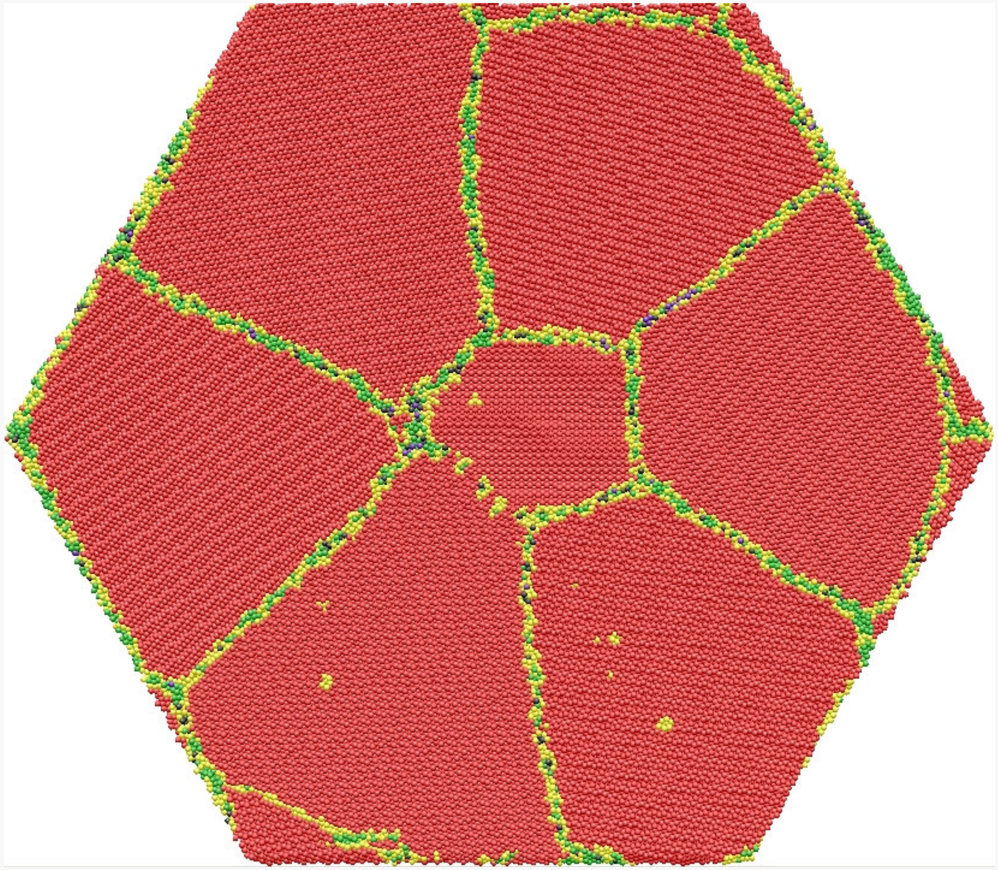
E_{PKA} = 5 keV at T = 900K

Heterogeneous irradiation of polycrystal

A cascades with the energy 8 keV were generated every 15 ps.

The location of the PKA was in the region nearby the central grain.

Effective dose rate about $3 \cdot 10^{7}$ s^{-1}.

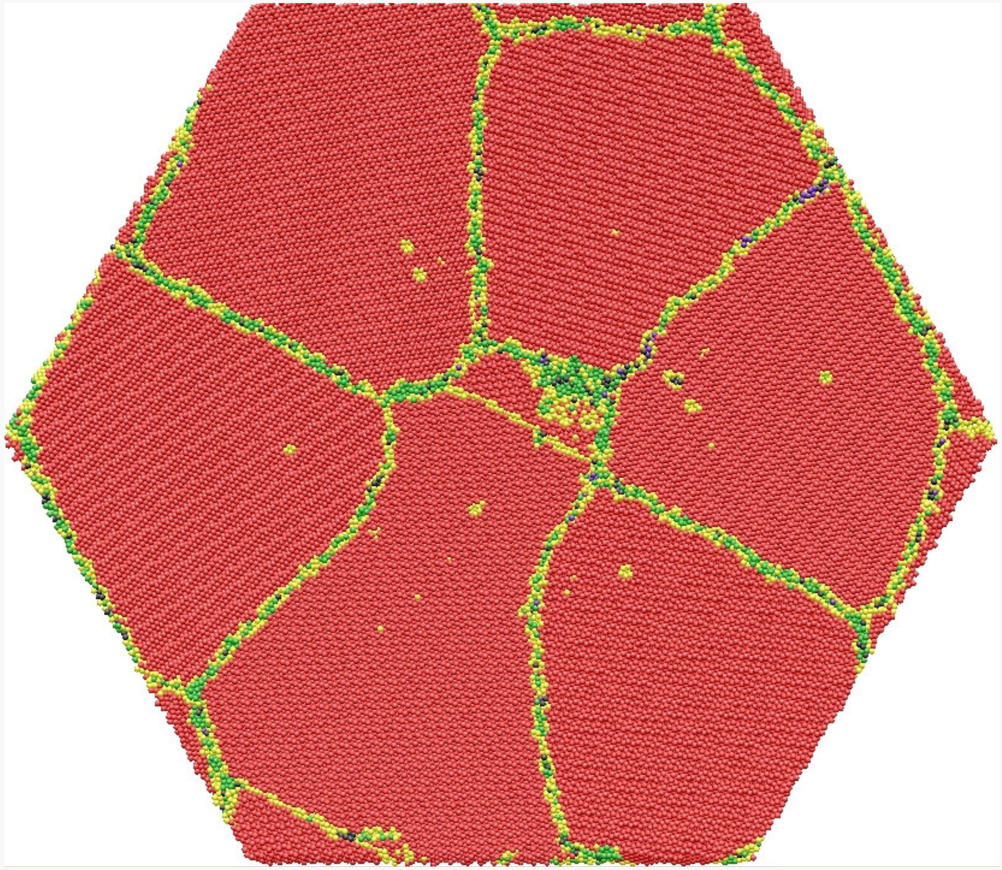


The polycrystal state after heterogeneous irradiation by 160 cascades with E_{PKA} = 8 keV at T = 900K

Heterogeneous irradiation of polycrystal

The dissolution of the central grain was observed

Effective irradiation dose of the central zone was about 0.15 dpa.



The polycrystal state after heterogeneous irradiation by 350 cascades with E_{PKA} = 8 keV at T = 900K

Conclusion

- *Biased creation of vacancies near the voids is observed both for low energy and high energy cascades.*

- *The defect formation in the vicinity of the helium bubbles shows the opposite picture namely the preferential formation of the interstitial atoms.*

- *The impact of heterogeneous irradiation on recrystallization processes in nanosize polycrystal is observed*