Displacement cascade database for PKA energies up to 50 keV in bcc-Fe

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Technical Meeting on A Database of Atomic Configurations Formed in Collision Cascades

IAEA Headquarters, Vienna, Austria

16 - 17 November 2017

CRIEPI
Central Research Institute of Electric Power Industry

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CASCADE DATABASE

Defect production in bcc-Fe

- Observation in low PKA energy cascades -

- Damage energy : Threshold energy ~ 100keV
- SIA-cluster (dislocation loop) formation occurs in the cascades with the PKA energies higher than 10keV.
- No definite clustering of vacancies.
- Sub-cascade formation in the cascades occurs with the PKA energies higher than 20keV.
- A very large diversity in high-energy cascade results.

What is the statistical characteristics?

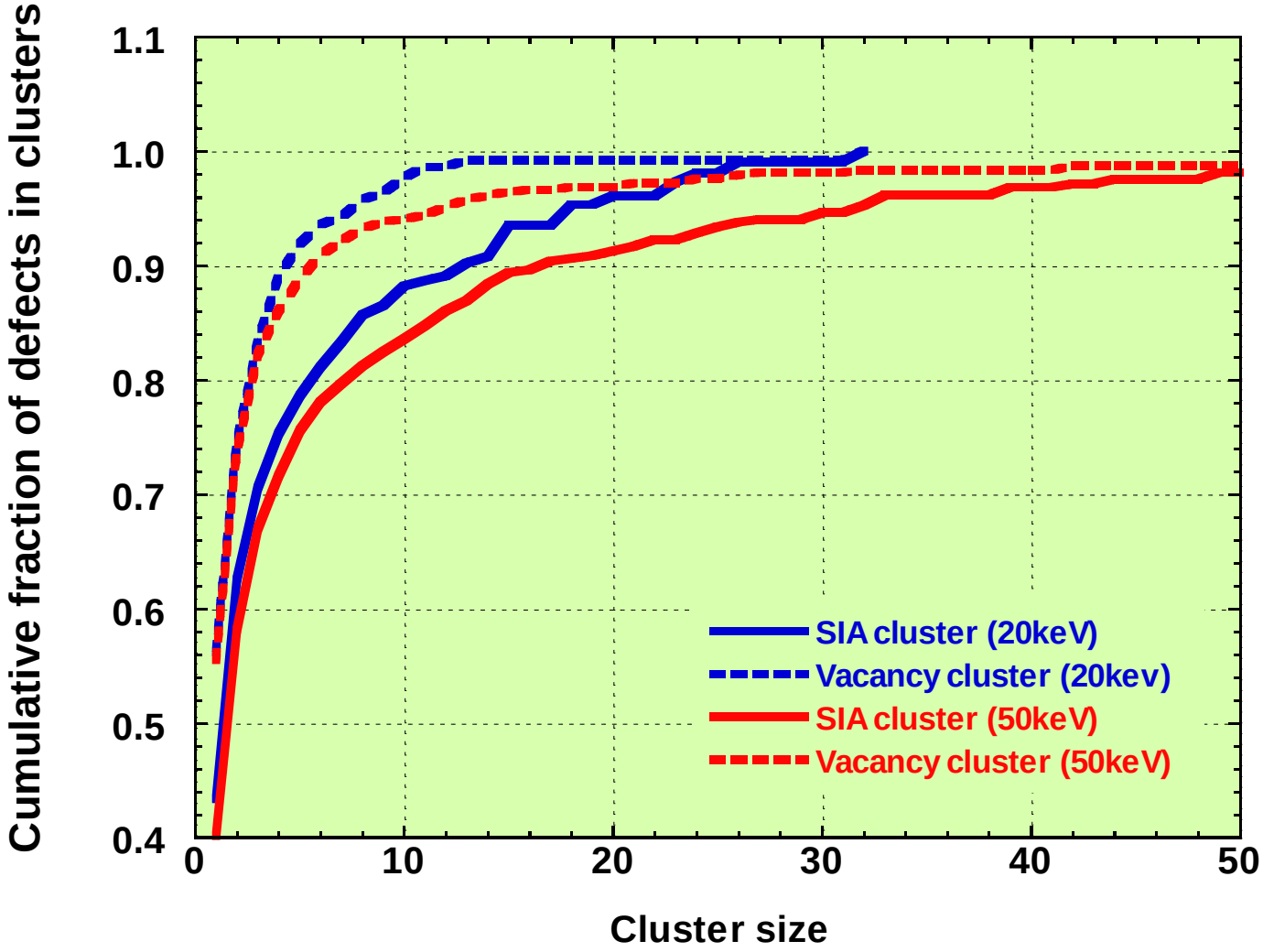
Objectives

- Characterize defect production due to high-energy cascade in bcc-Fe by performing a number of Molecular Dynamics (MD) calculations
  - 100 runs of 50keV cascade
  - 50 runs of 20keV cascade

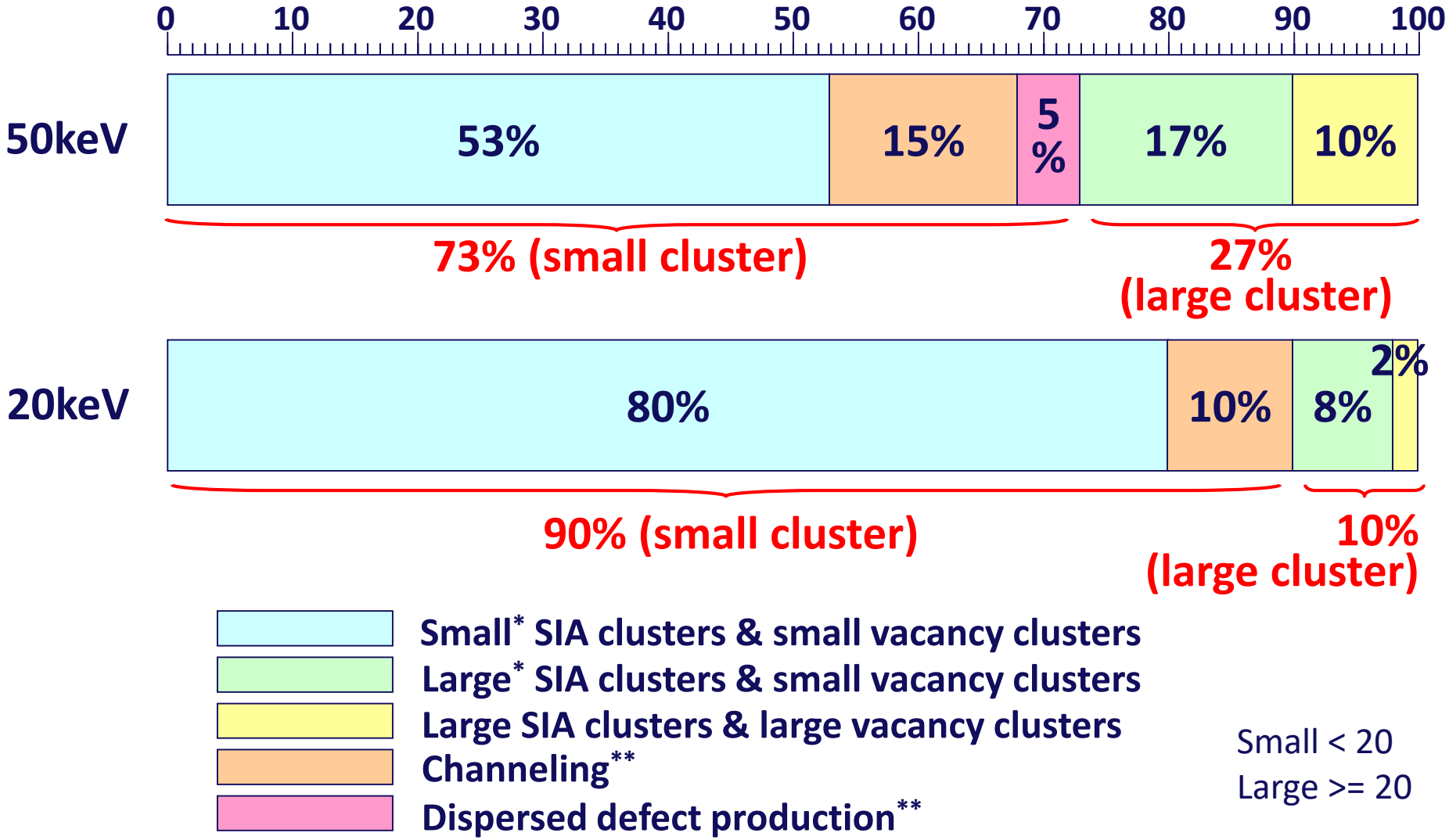
Calculation

- Johnson & Oh's EAM potential
  - ZBL universal potential in a short ranage
- Computation box
  - 2,000,000 ($2x100^3$) atoms for 50keV cascades
  - 1,024,000 ($2x80^3$) atoms for 20keV cascades
- Crystal temperature : 600K
- Constant volume
- No electron-phonon coupling
- Clustering criteria :
  - 3NN for SIA clusters
  - 4NN for Vacancy clusters

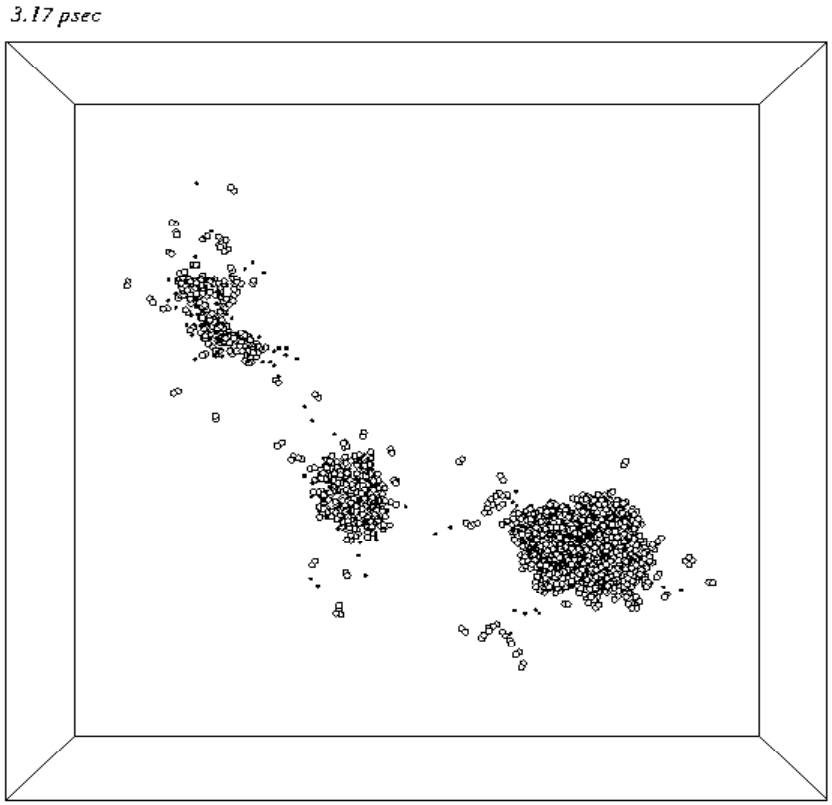
Fraction of defects in clusters

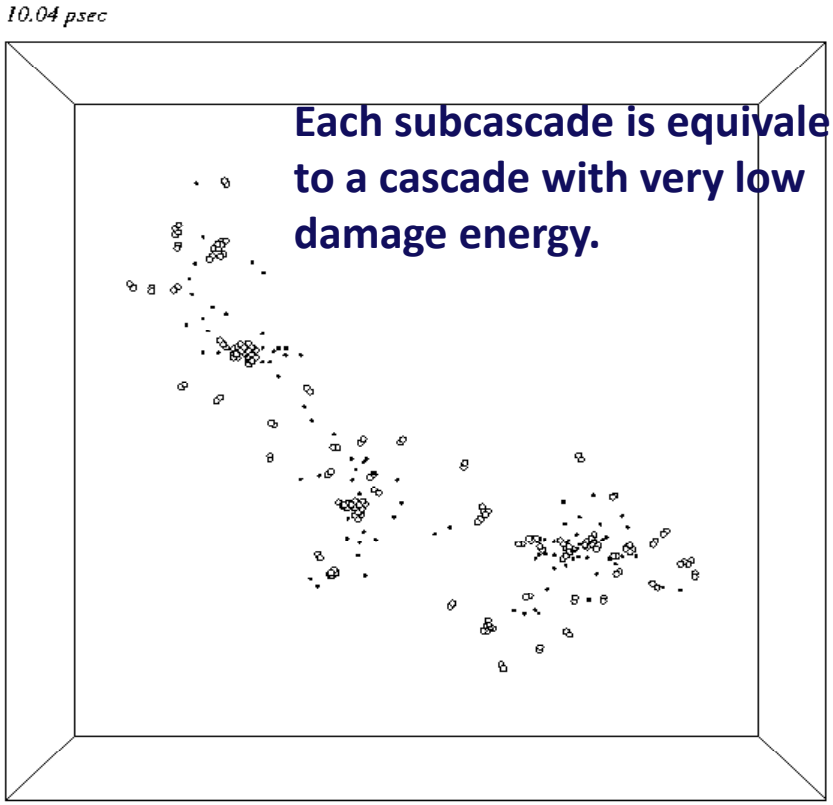


Classification of defect formation again



Small SIA & small vacancy cluster





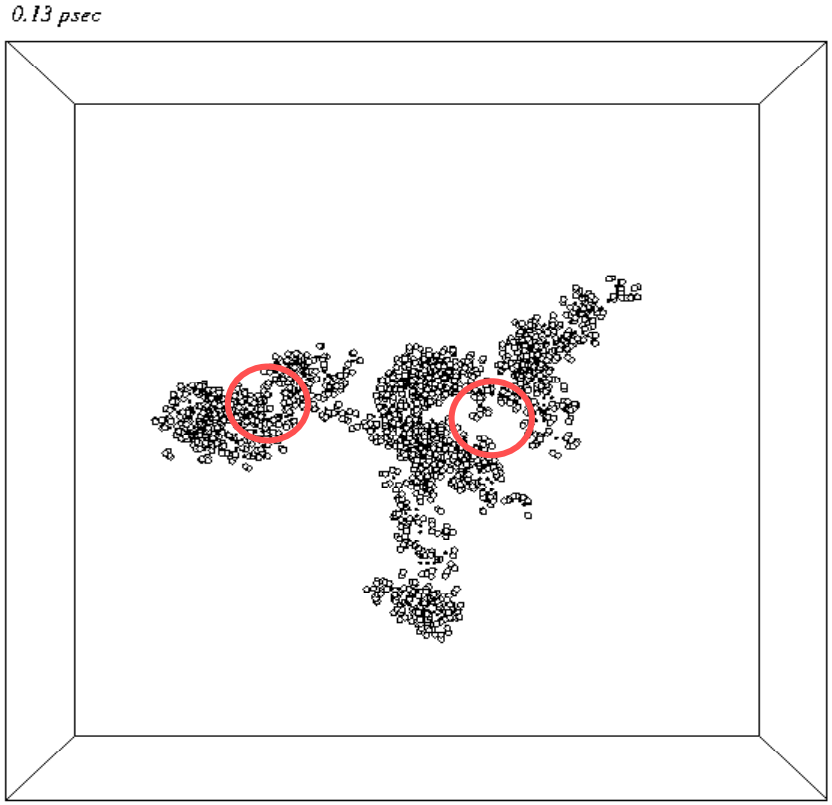
Each subcascade is equivalent to a cascade with very low damage energy.

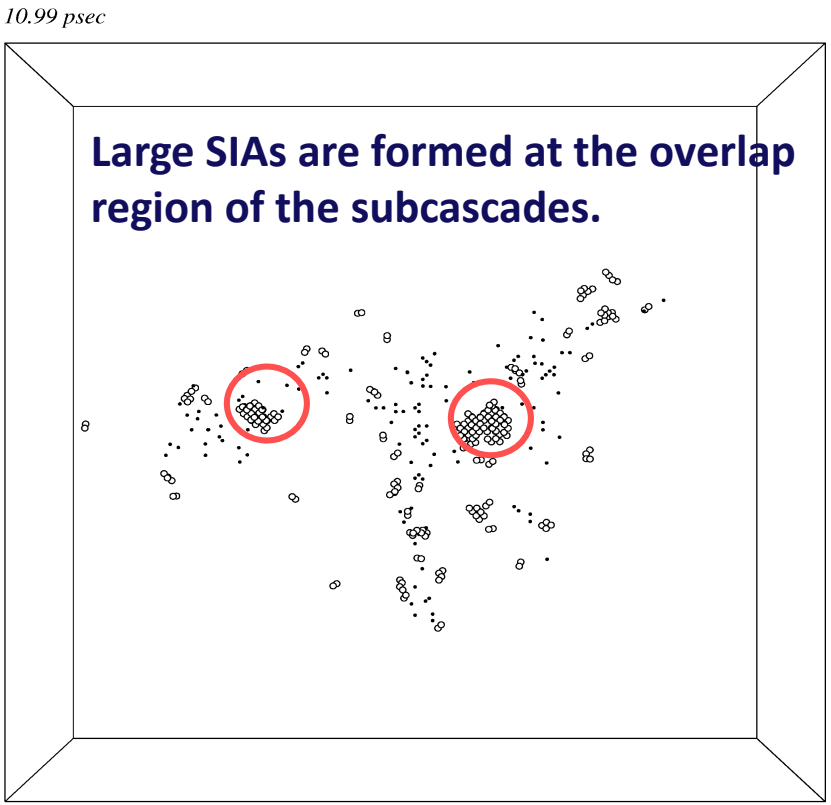
Isolated subcascades

Black dots : vacancies
White circles : SIAs

Case 45

Large SIA & small vacancy cluster



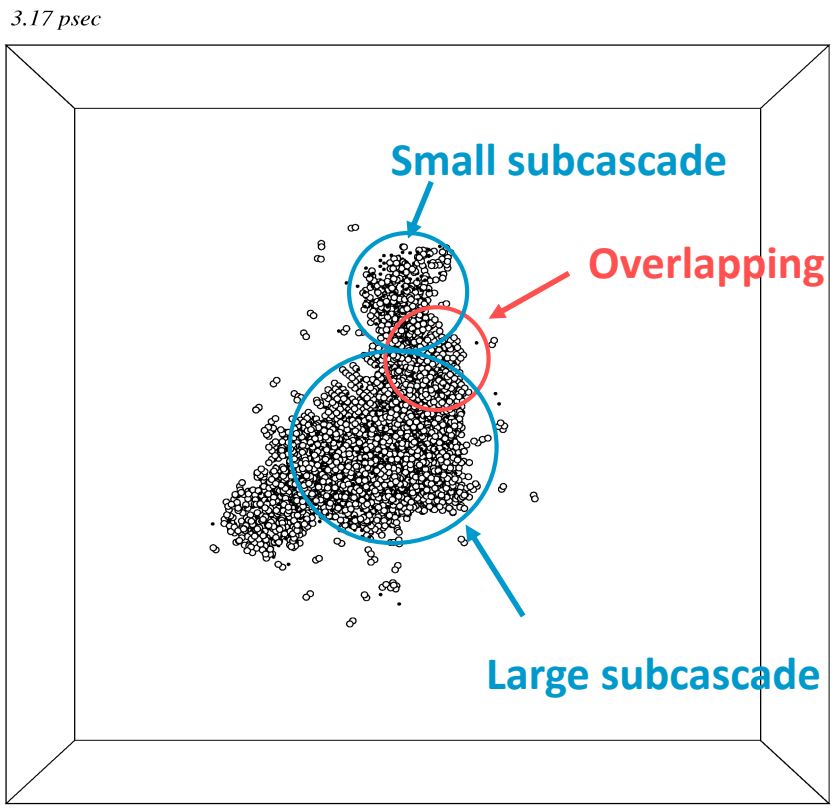


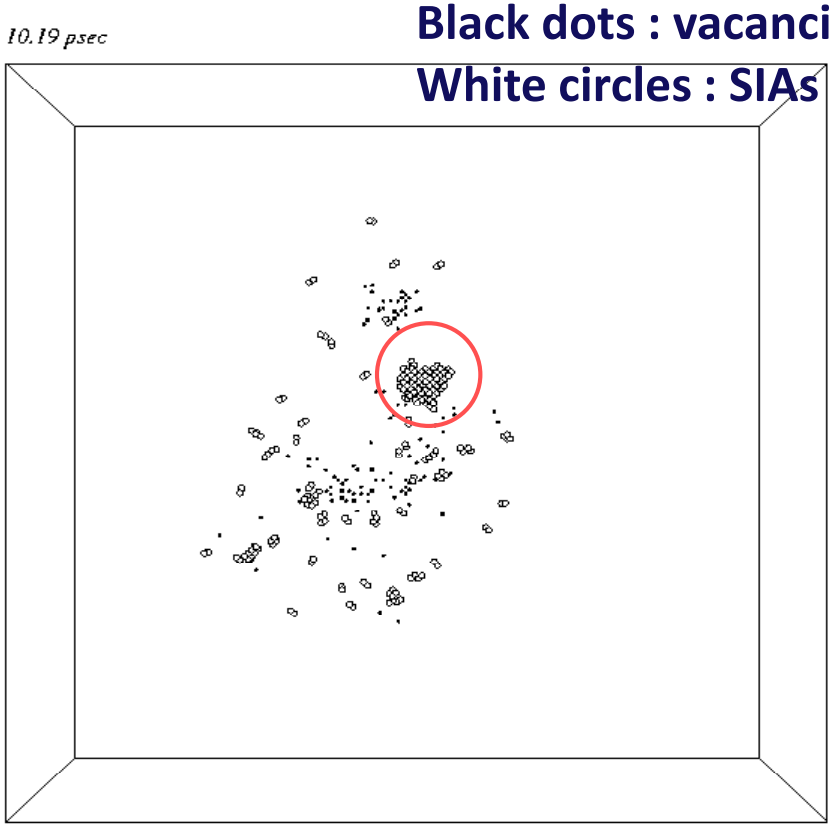
Overlapping of subcascades of similar sizes

Black dots : vacancies
White circles : SIAs

Case 09

Large SIA & large vacancy cluster (1)





Black dots : vacancies

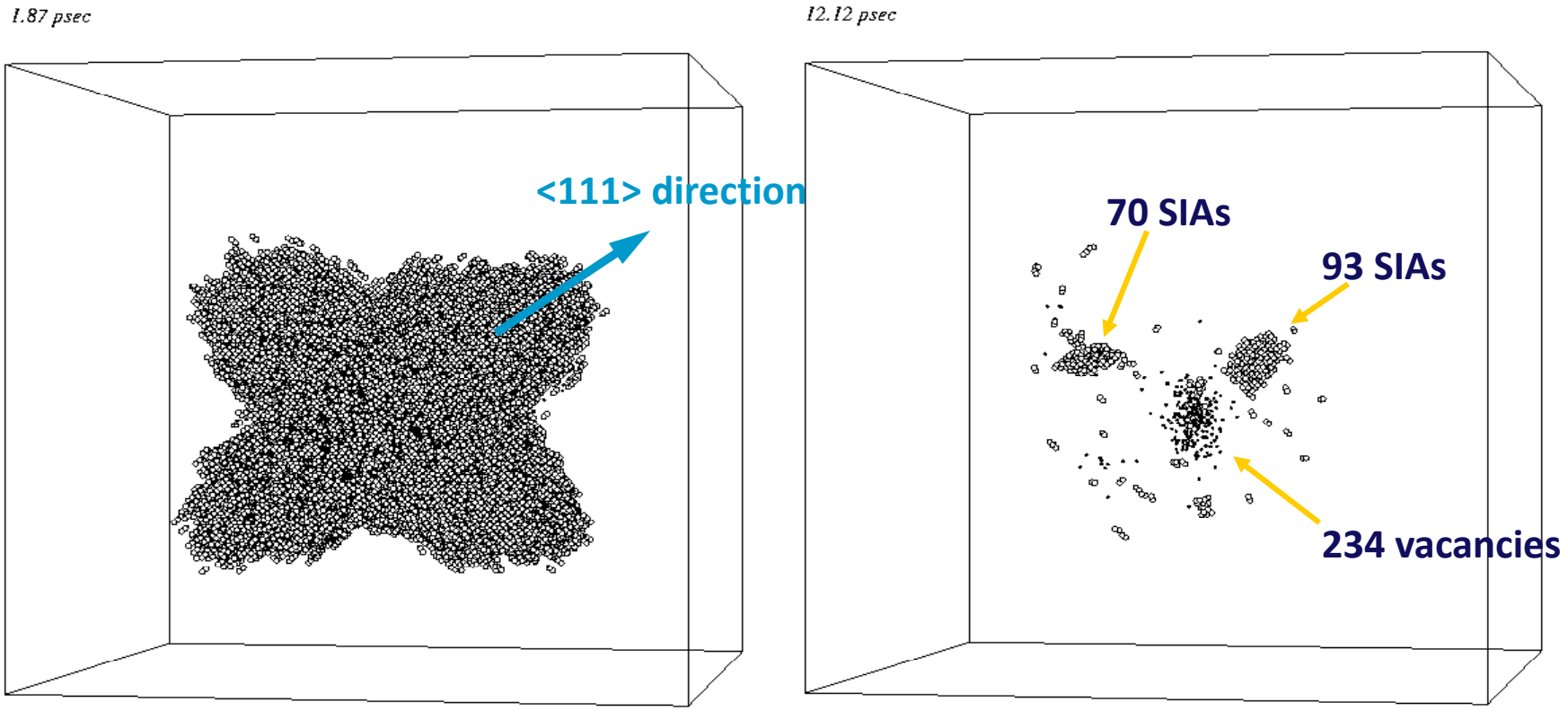
White circles : SIAs

Overlapping of subcascades of different sizes

- A very large SIA cluster is formed at the overlap of large and small subcascades.
- Consequently, many vacancies are left particularly at the core of the larger subcascade.

Case 28

Large SIA & large vacancy cluster (2)

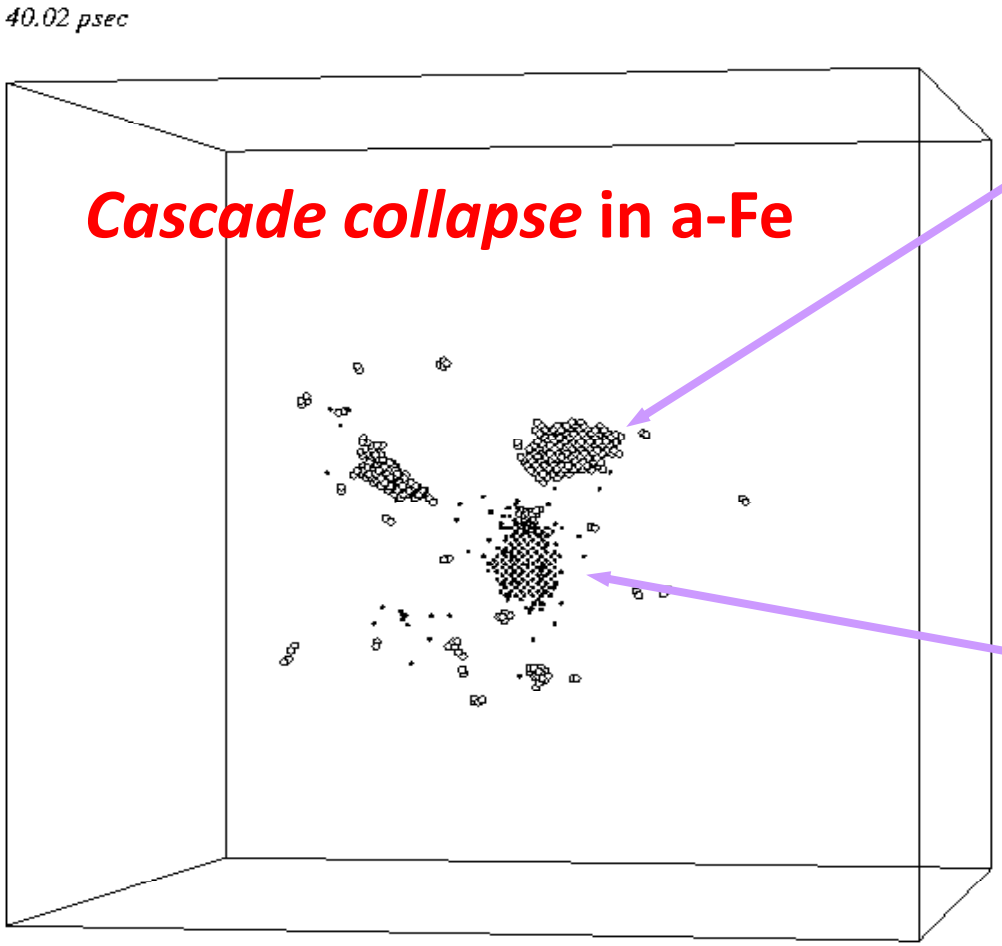


One large cascade, and then …

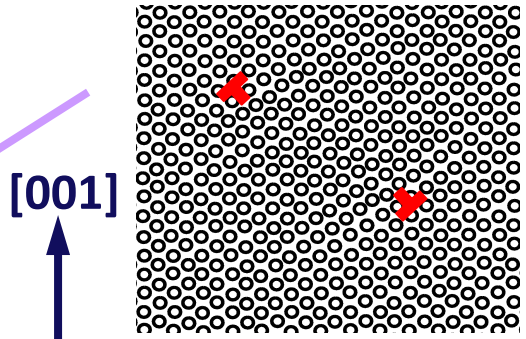
Black dots : vacancies
White circles : SIAs

Case 39

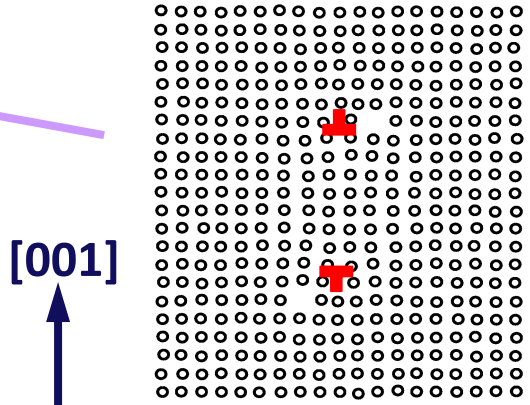
Large SIA & large vacancy cluster (3)



Black dots : vacancies
White circles : SIAs



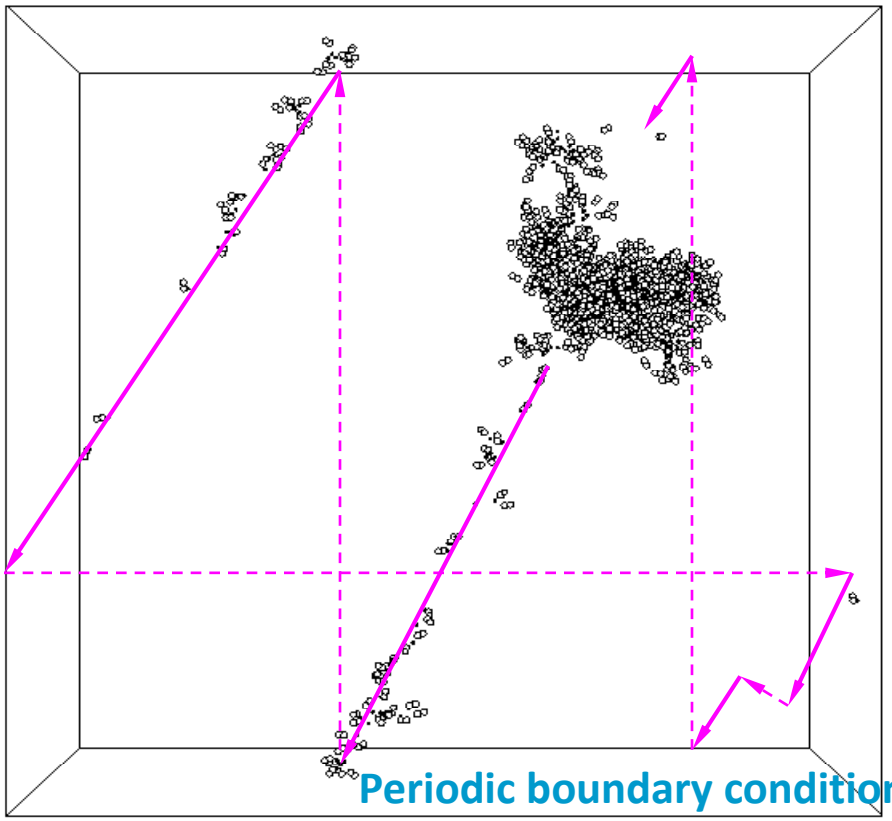
Large SIA loop
b = $a_0/2$ <111>



Large vacancy loop
b = a_0 <100>

Case 39

Channeling



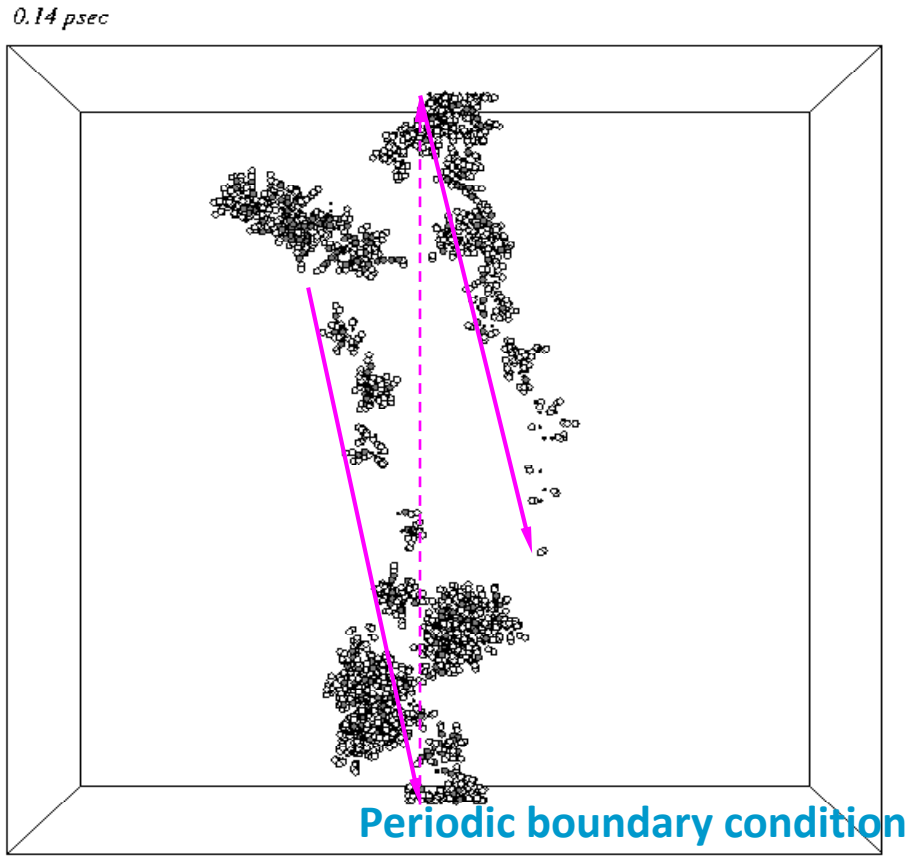
Black dots : vacancies
White circles : SIAs

Direction	50keV	20keV
⟨011⟩	2	0
⟨133⟩	1	0
⟨233⟩	2	0
⟨111⟩	0	1
⟨112⟩	1	1
⟨337⟩	1	0
⟨113⟩	1	0
⟨114⟩	1	0
⟨115⟩	0	1
⟨116⟩	1	2
⟨001⟩	7	0

- All the events occur on (110) plane.
- PKA is always the channel particle in 20keV cascades.

Case 31

Dispersed defect production



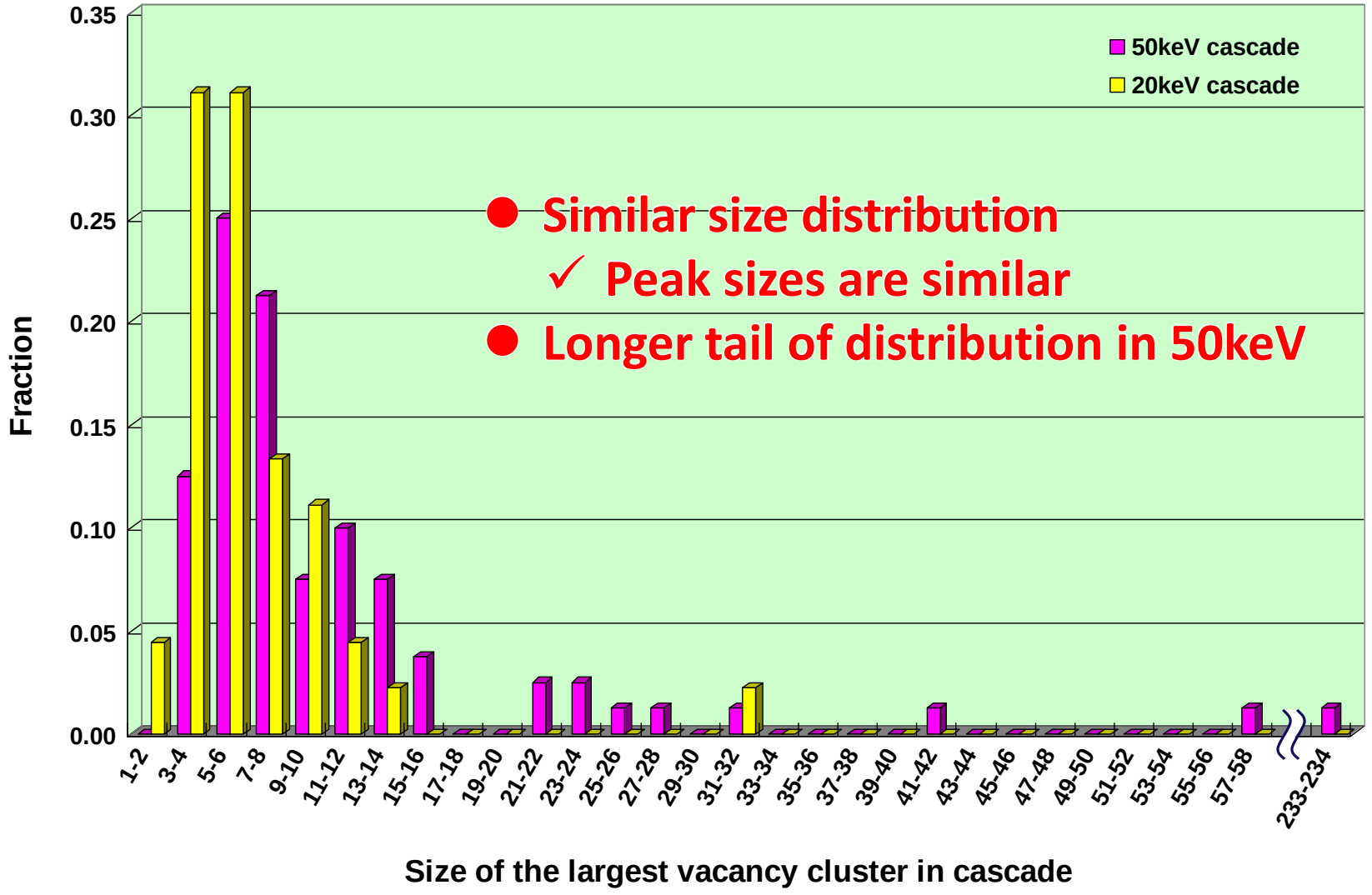
Black dots : vacancies
White circles : SIAs
Gray : replaced atoms

Case 42

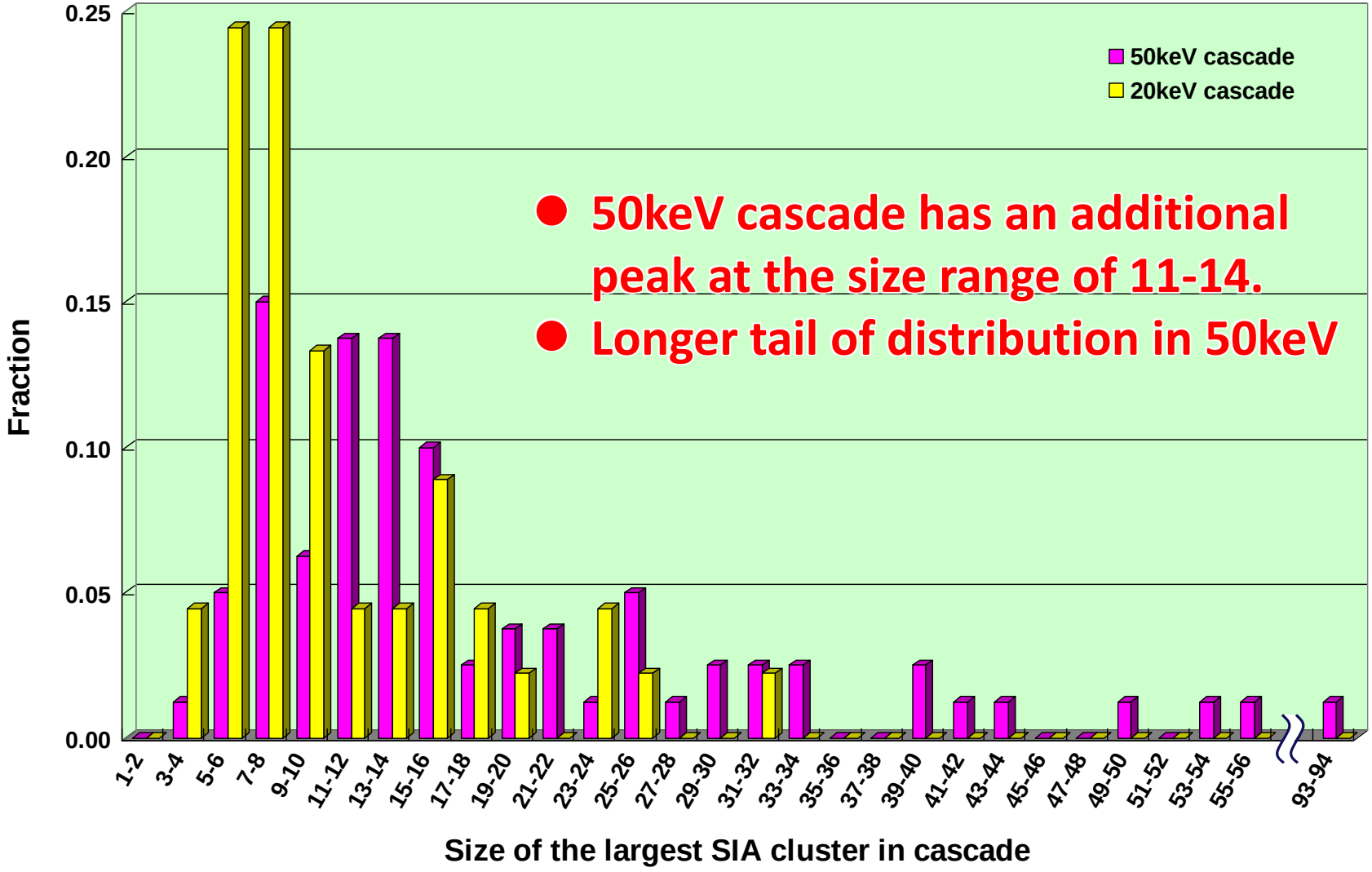
Direction	50keV	20keV
⟨011⟩	1	0
⟨111⟩	1	0
⟨113⟩	2	0
⟨001⟩	1	0

- Similar direction to channeling, but associated with many interactions
- Did not occur in 20keV cascades

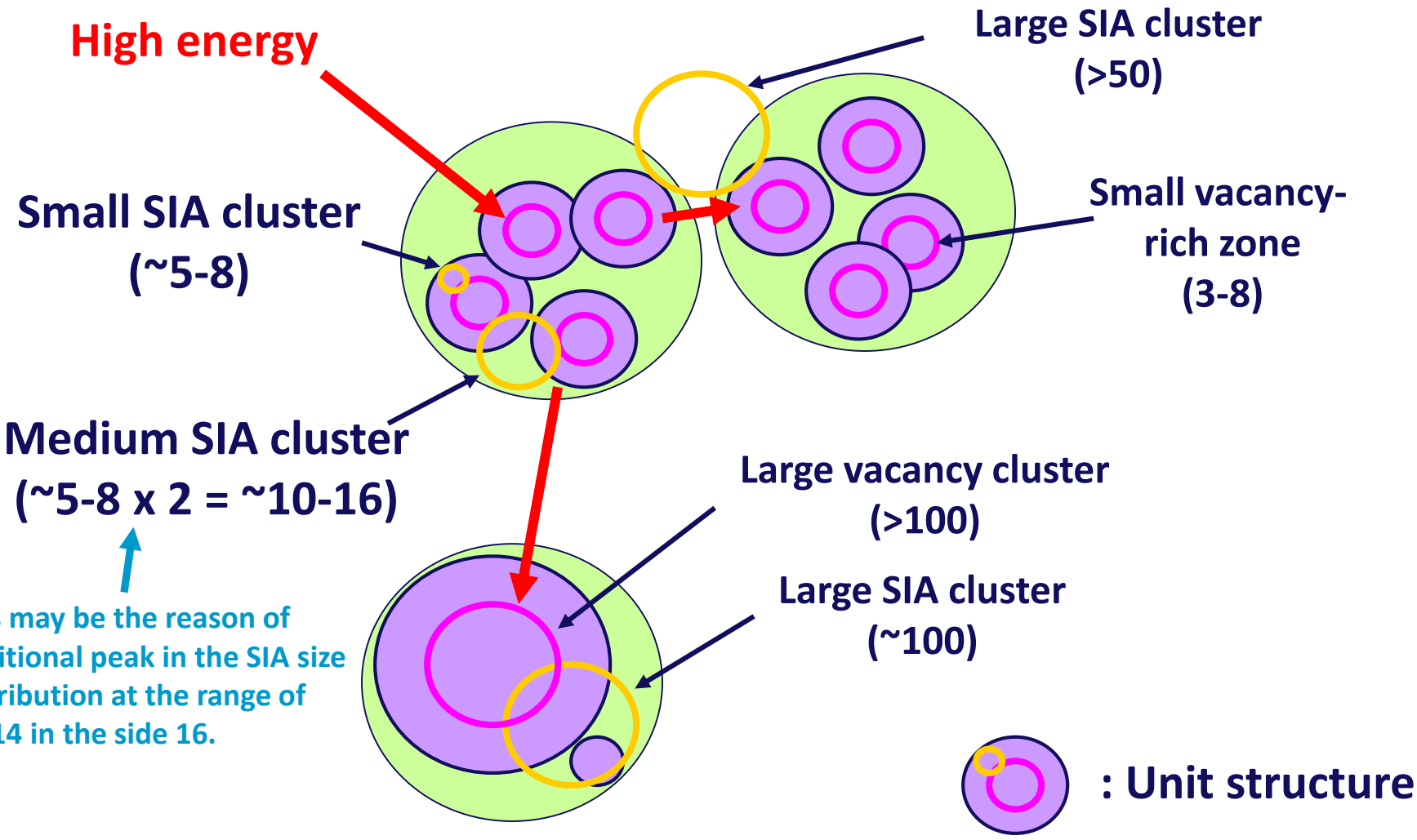
Structure of cascades – vacancy –



Structure of cascades – SIA –

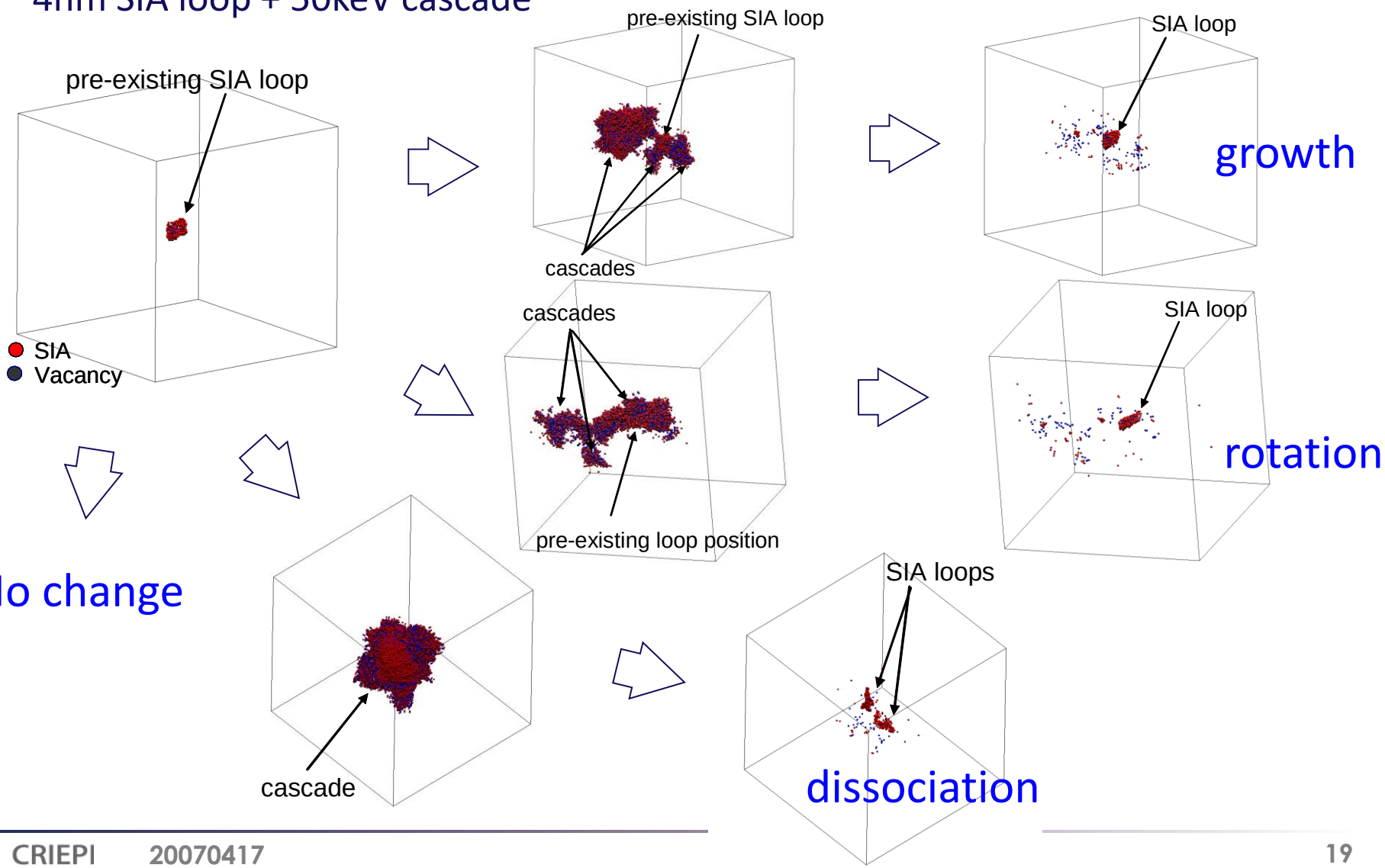


Structure of cascade

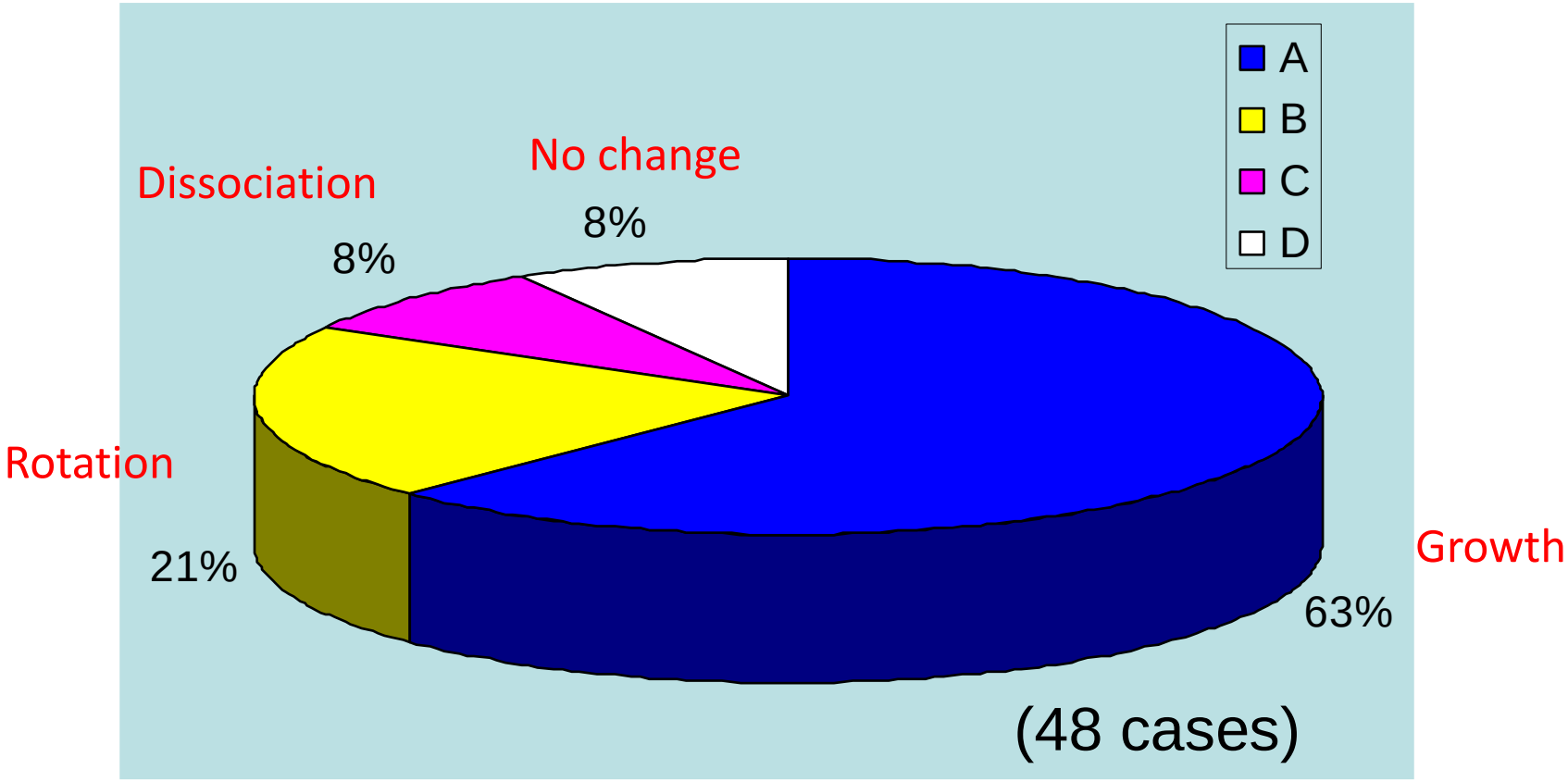


Cascade-overlap at high doses

4nm SIA loop + 50keV cascade



Cascade overlap statistics



Conclusions

- Both 50keV and 20keV cascades basically provide small point defect clusters. In 50keV cascade, however, there is a relatively large chance to produce large SIA clusters (~30%) and large vacancy clusters (~10%). These large defect clusters may play an important role in the microstructure evolution.
- “Cascade collapse” in bcc-Fe was observed for the first time by molecular dynamics simulation. 1/100 probability looks consistent with the low defect yield in bcc-Fe in experiments.
- 50keV and 20keV cascades consist of very similar unit structure (small subcascade).

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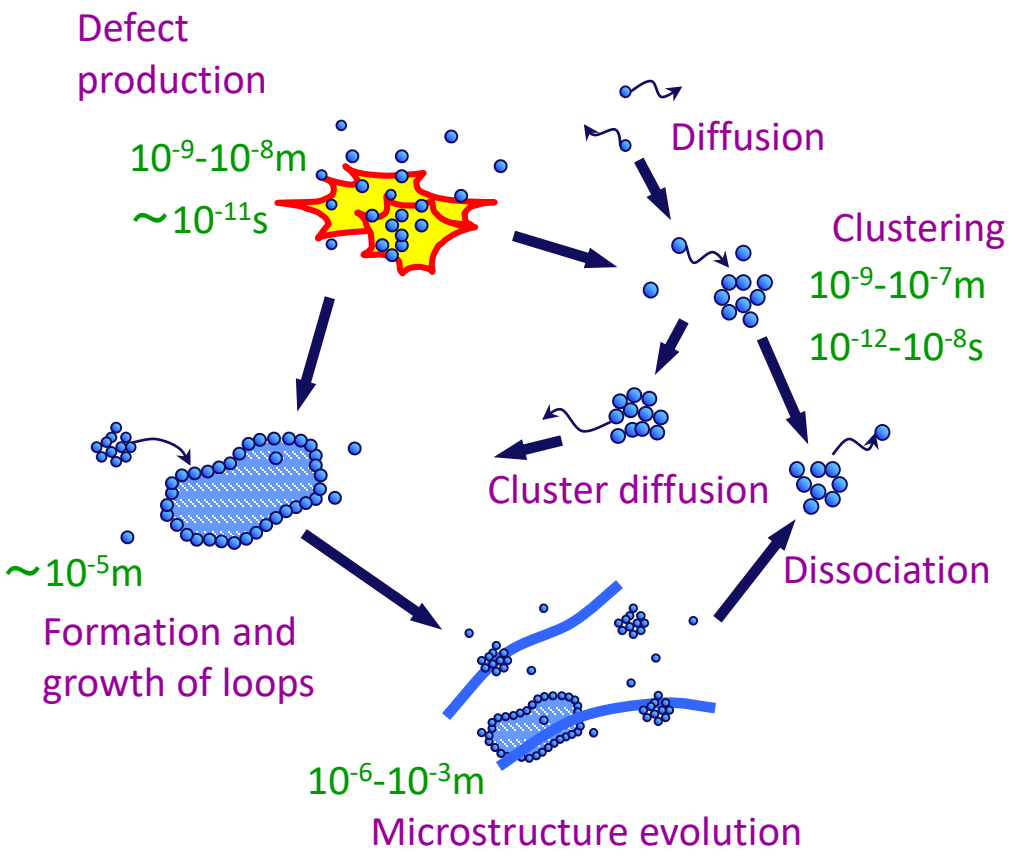
KINETIC MONTE CARLO SIMULATIONS USING CASCADE DATABASE

Objectives

- Effect of PKA energy spectrum
- Effect of irradiation temperature
- Effect of dose rate

Outline of KMC

KMC tracks all the events.



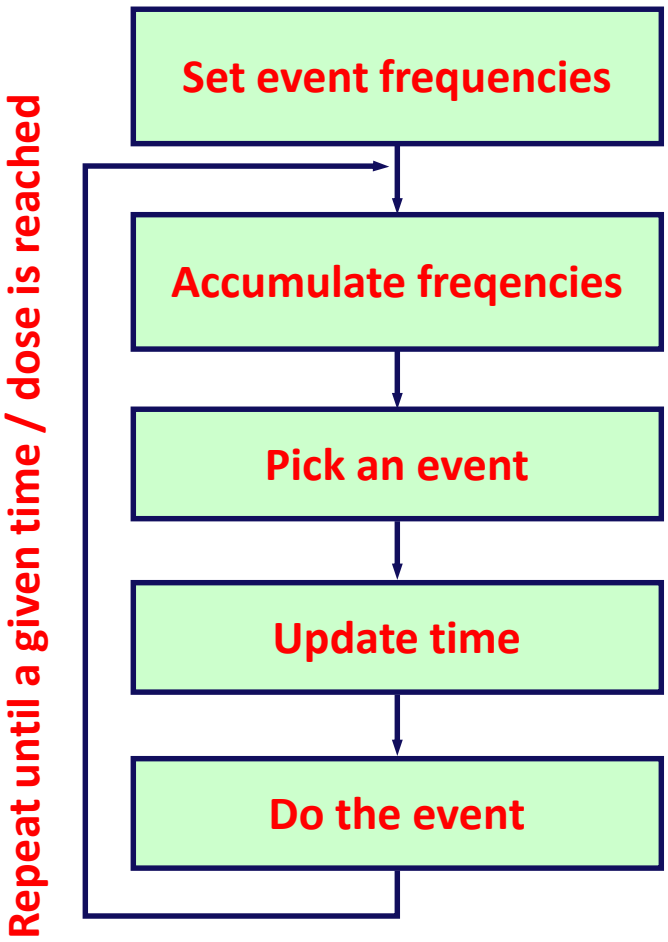
Input Data

- Database of displacement cascades for a wide range of PKA energies
- Diffusion kinetics such as diffusivities and diffusion modes (1D, 3D…) of point defects and clusters
- Thermal stabilities (binding energies) of point defect clusters

Most of the data can be obtained from molecular dynamics simulations.

KMC Algorithm

Particles & Events



Diffusion → D_o, E_m

Dissociation → D_o, E_b+E_m

Cascade → dose rate

$$P = \sum_i N_i P_i$$

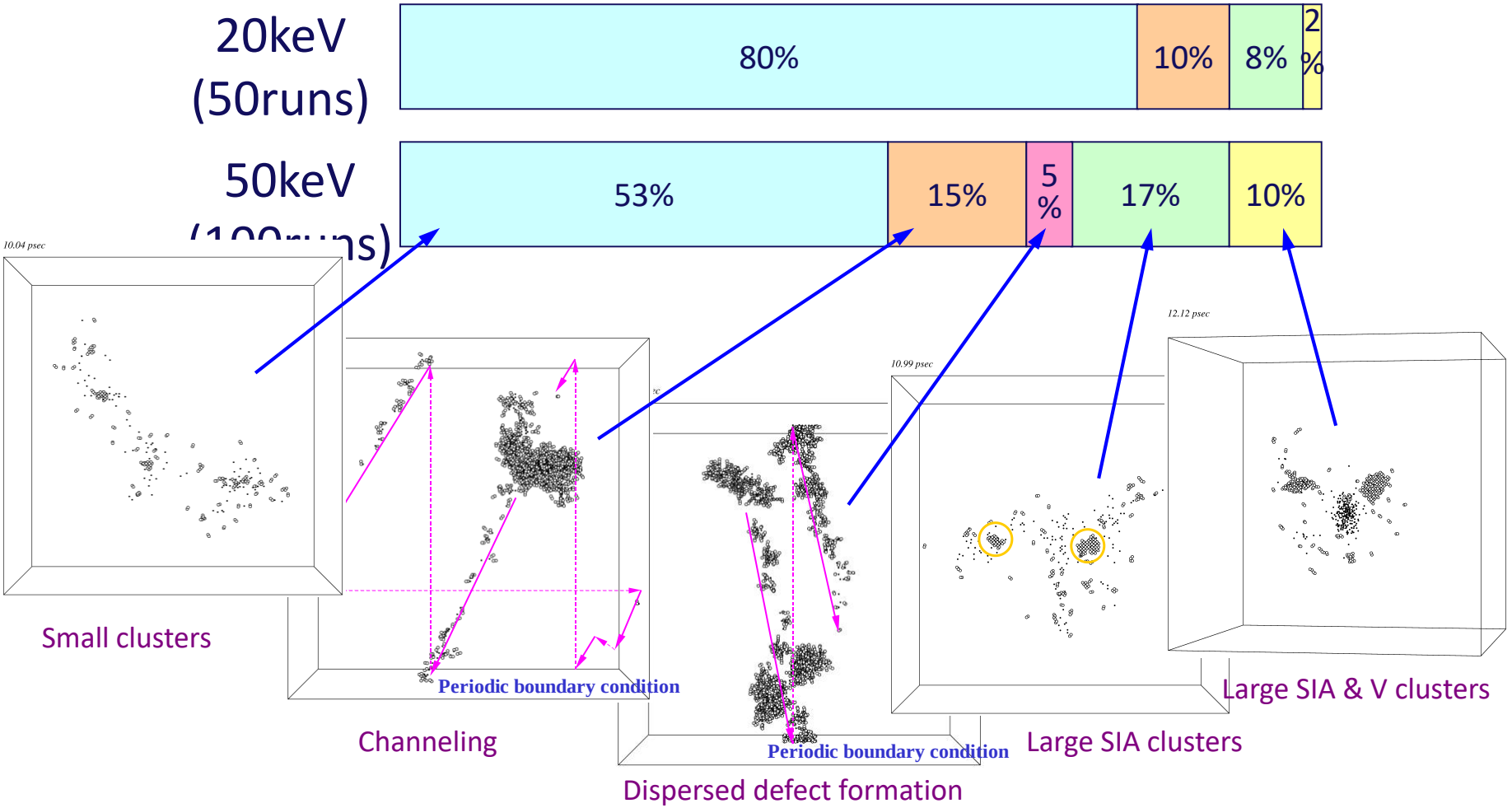
R = Random()*P

t = -log(R) / P

Interactions between enighboring particles (clustering, annihilation, etc.)

Displacement Cascade Database of bcc-Fe

PKA energies: 100eV, 200eV, 500eV, 1keV, 2keV, 5keV, 10keV, 20keV, 50keV

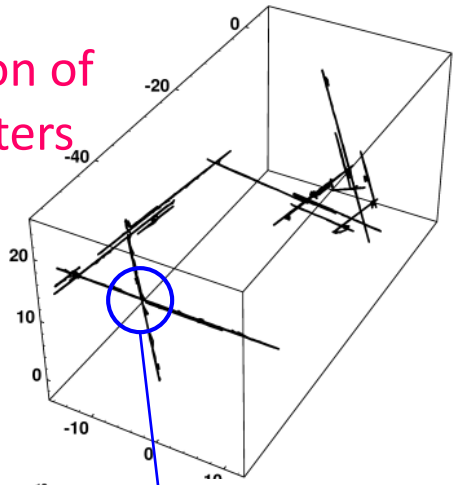


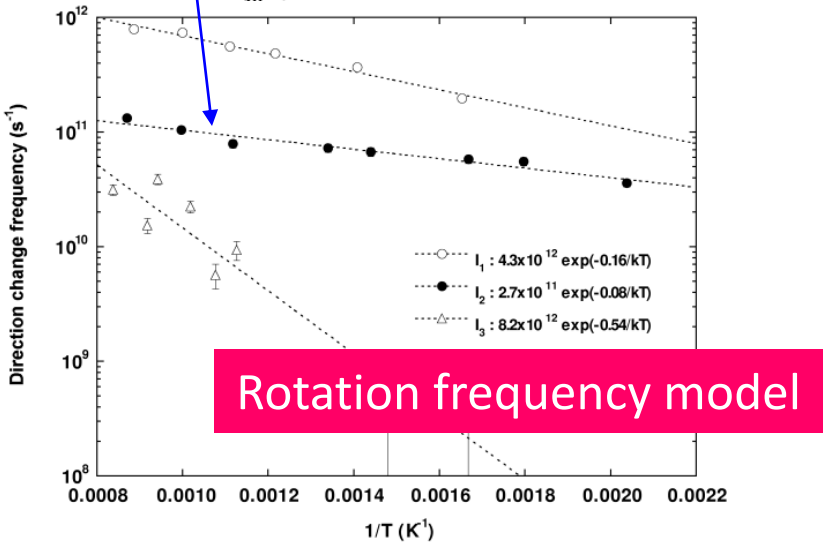
Cascade Database → Simulation of PKA Spectrum

N. Soneda, T. Diaz de la Rubia, S. Ishino, Phil. Mag. Letters, **81** (2001) 649.

Diffusion Kinetics of Point Defects in bcc-Fe

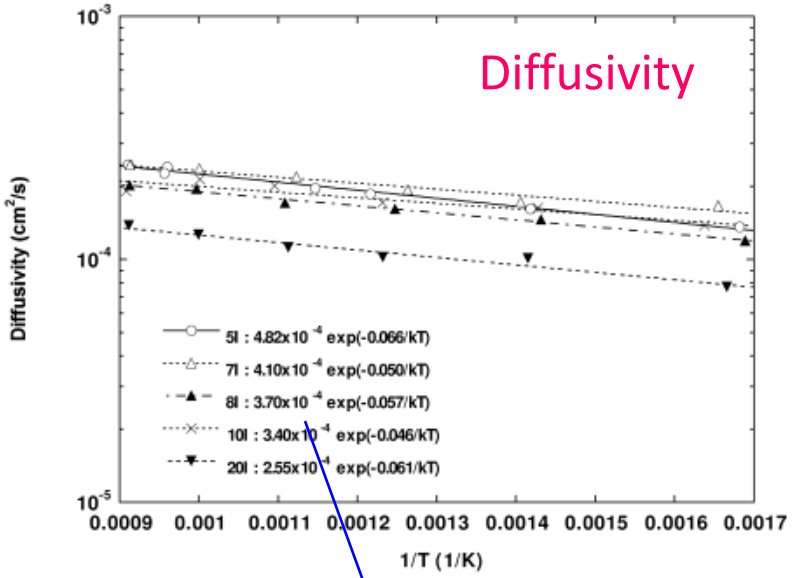
1D motion of SIA clusters



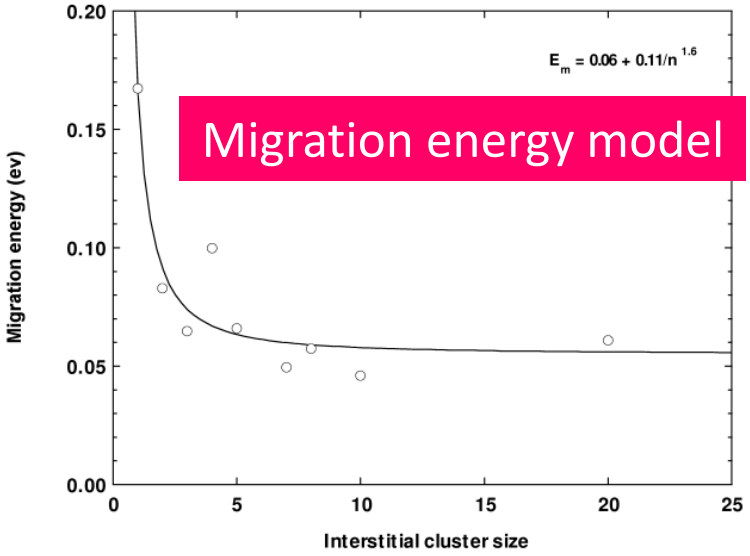


Rotation frequency model

Diffusivity



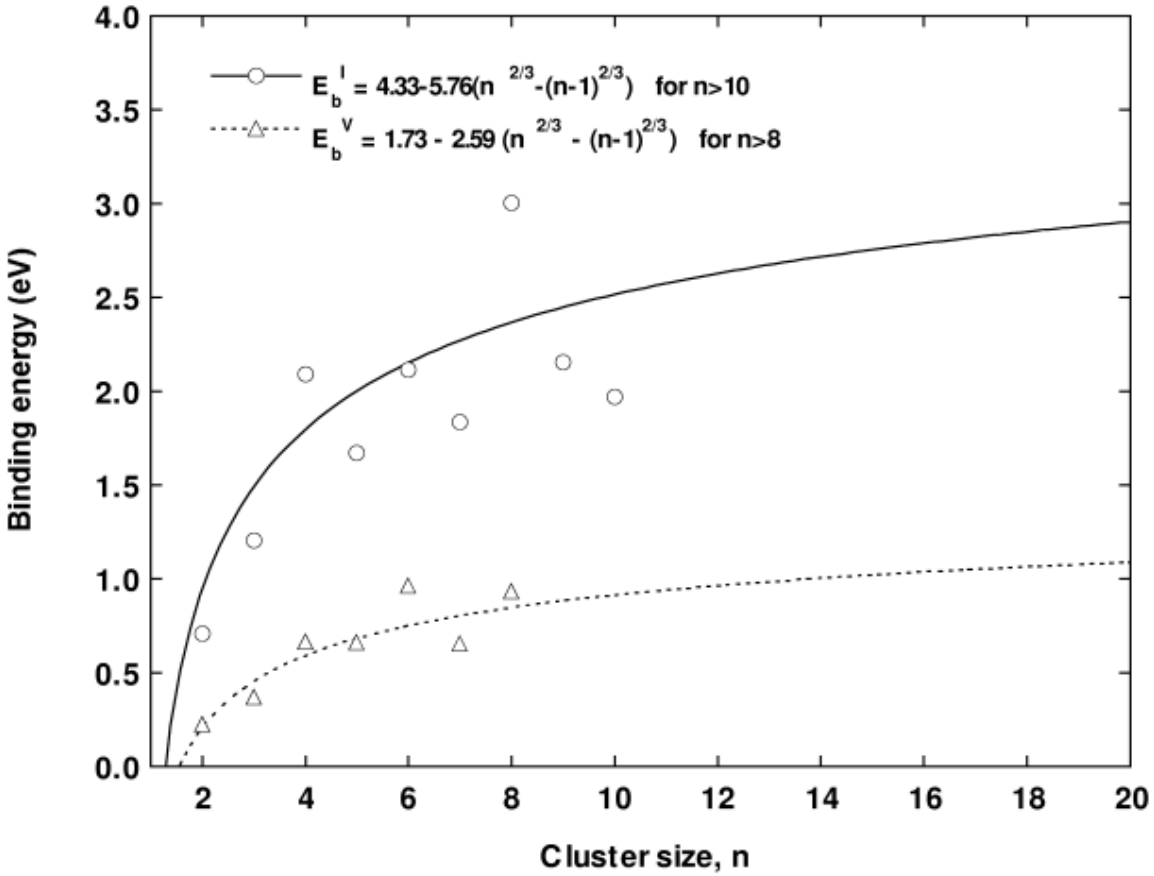
Migration energy model



N. Soneda, T. Diaz de la Rubia, Phil. Mag. A, **81** (2001), 331.

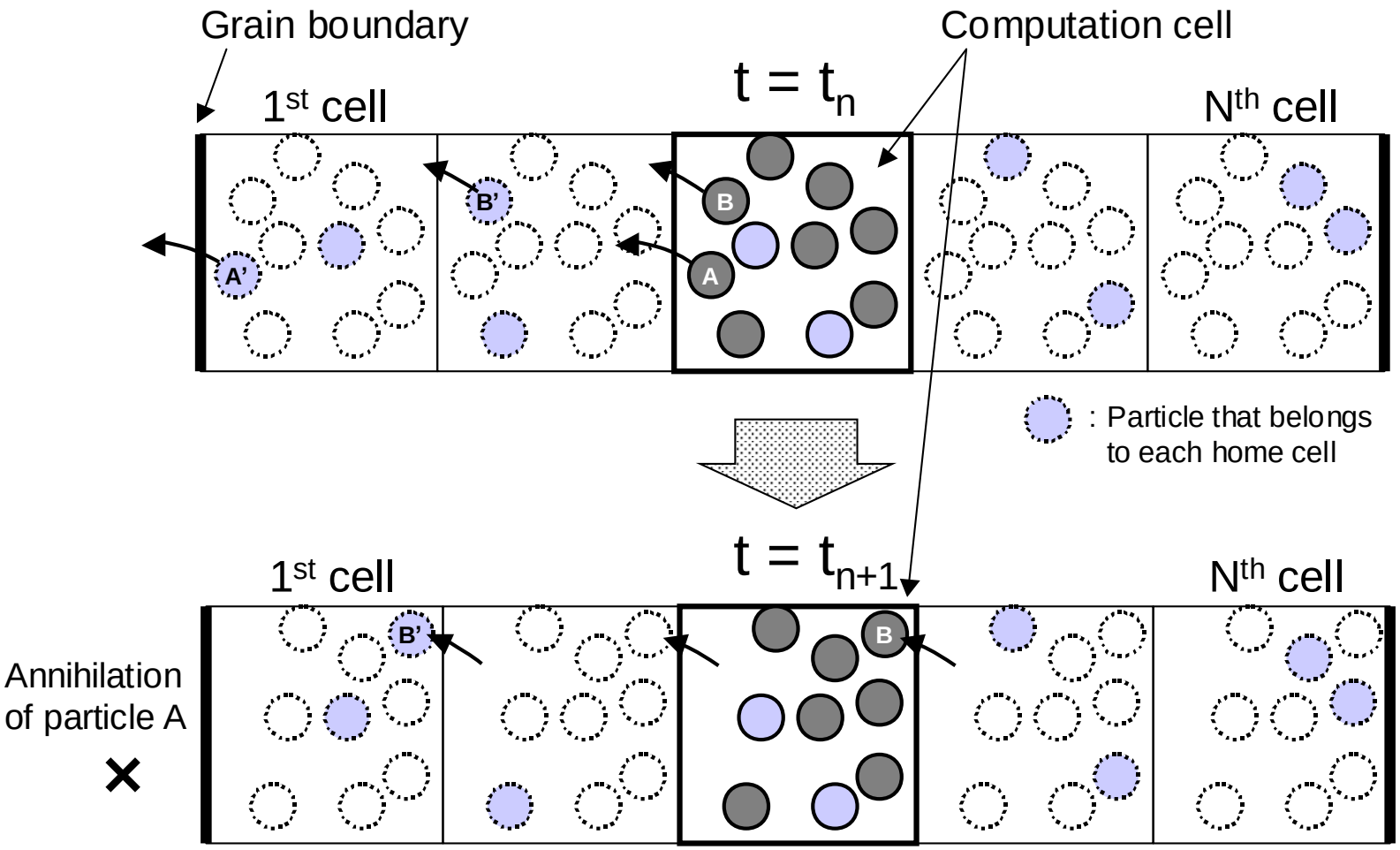
Binding Energies of Defect Clusters in bcc-Fe

Binding energy model

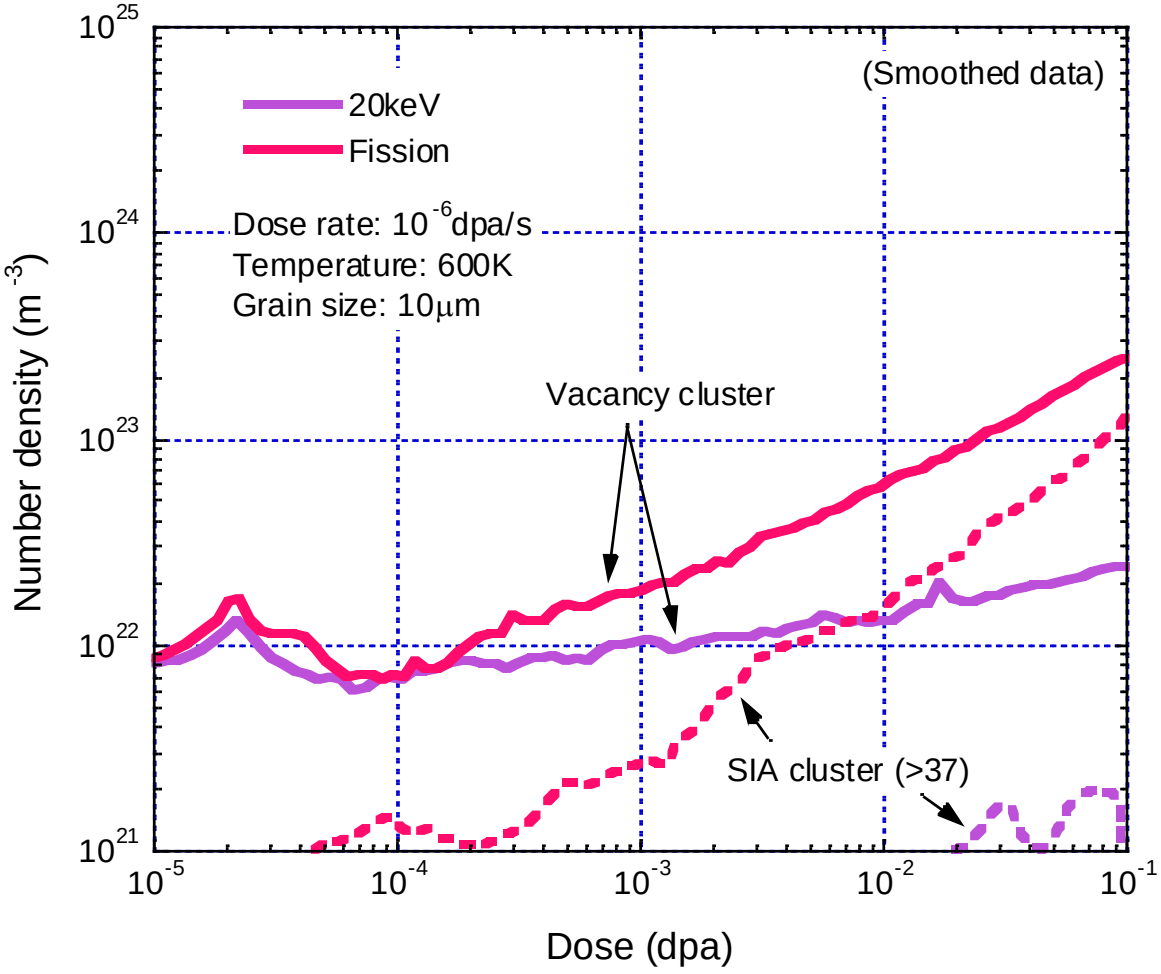


N. Soneda, T. Diaz de la Rubia, Phil. Mag. A, **78** (1998), 995.

Finite Periodic Boundary Condition

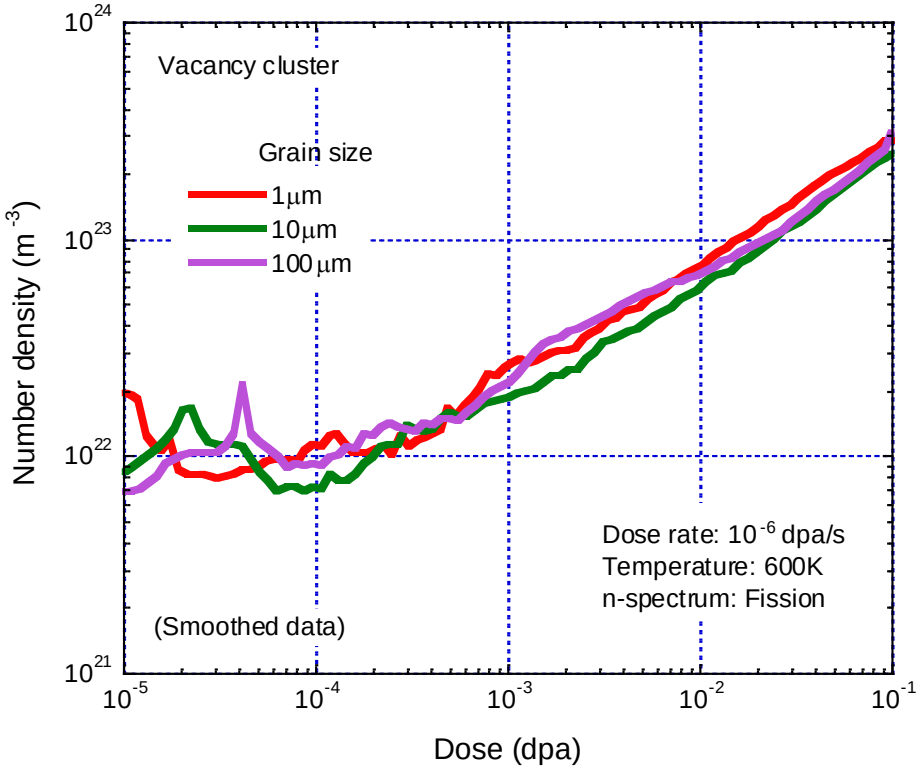


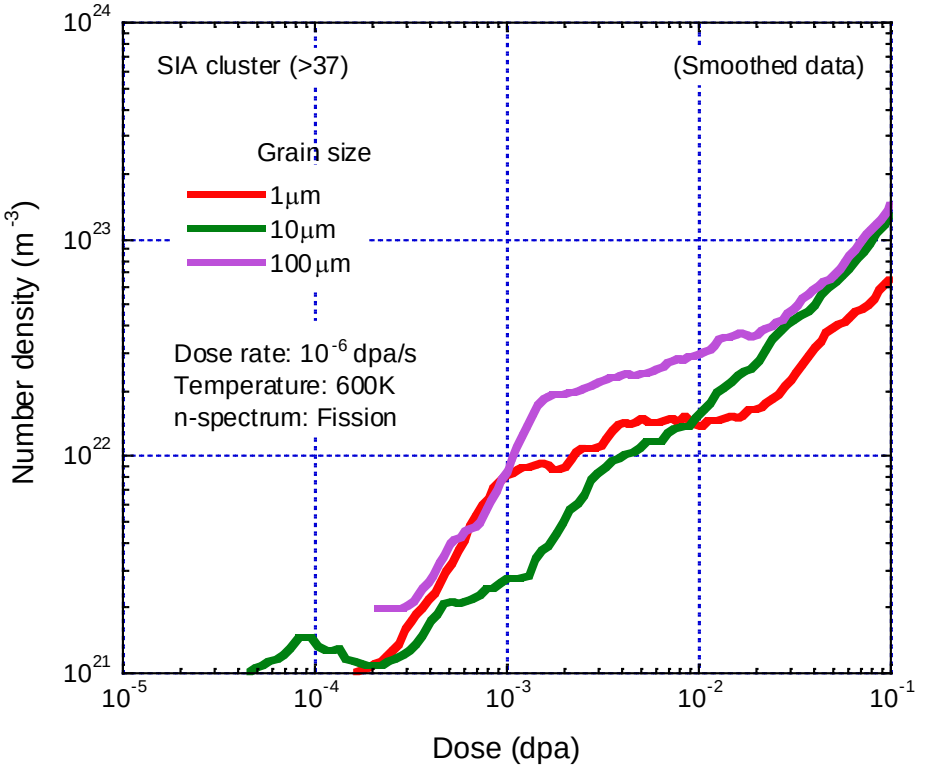
Effect of Neutron Spectrum



Direct formation of large clusters in cascades looks the key

Effect of Grain Size



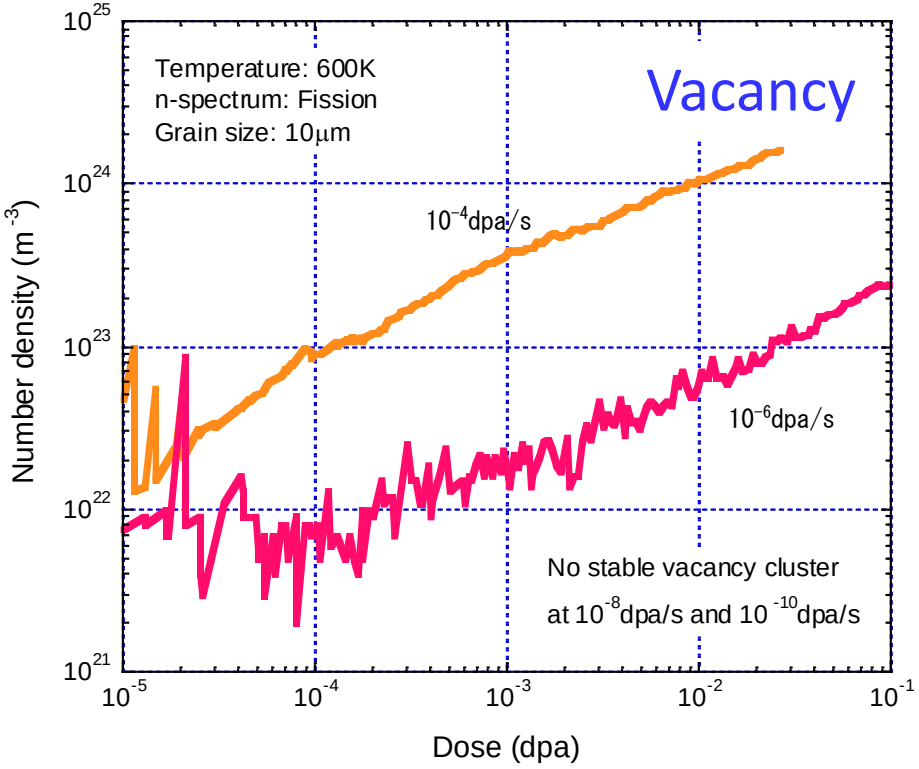


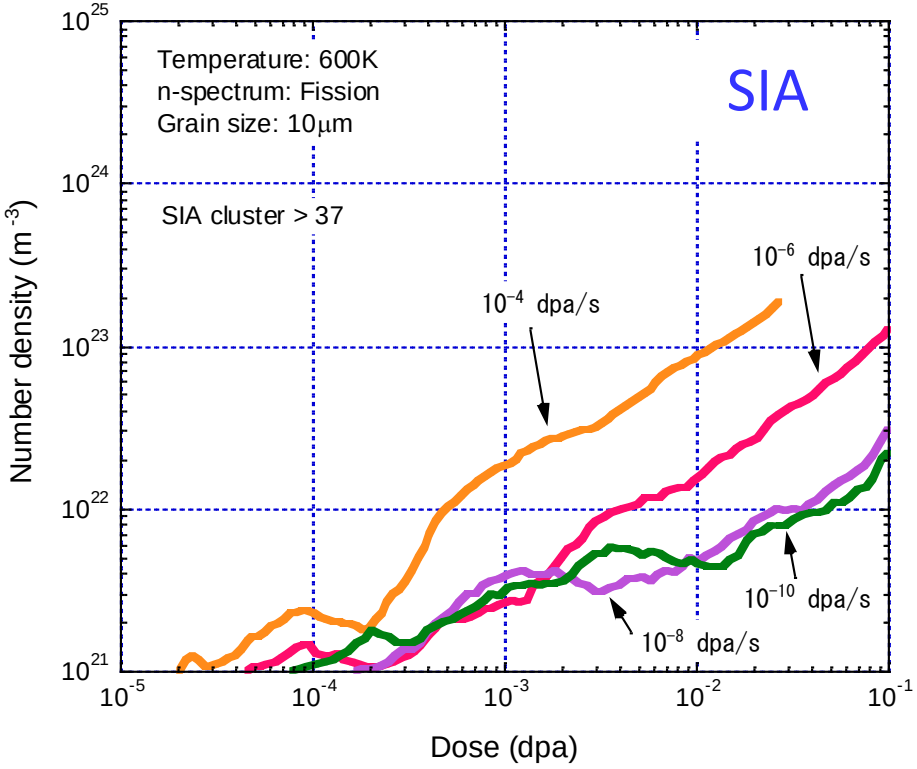
No effect

Small differences maybe due to the relationship between the length of mean free path of 1D-diffusing SIAs and the grain size

Dose Rate Effect in bcc-Fe

600K, Pure Fe, fast n-irradiation

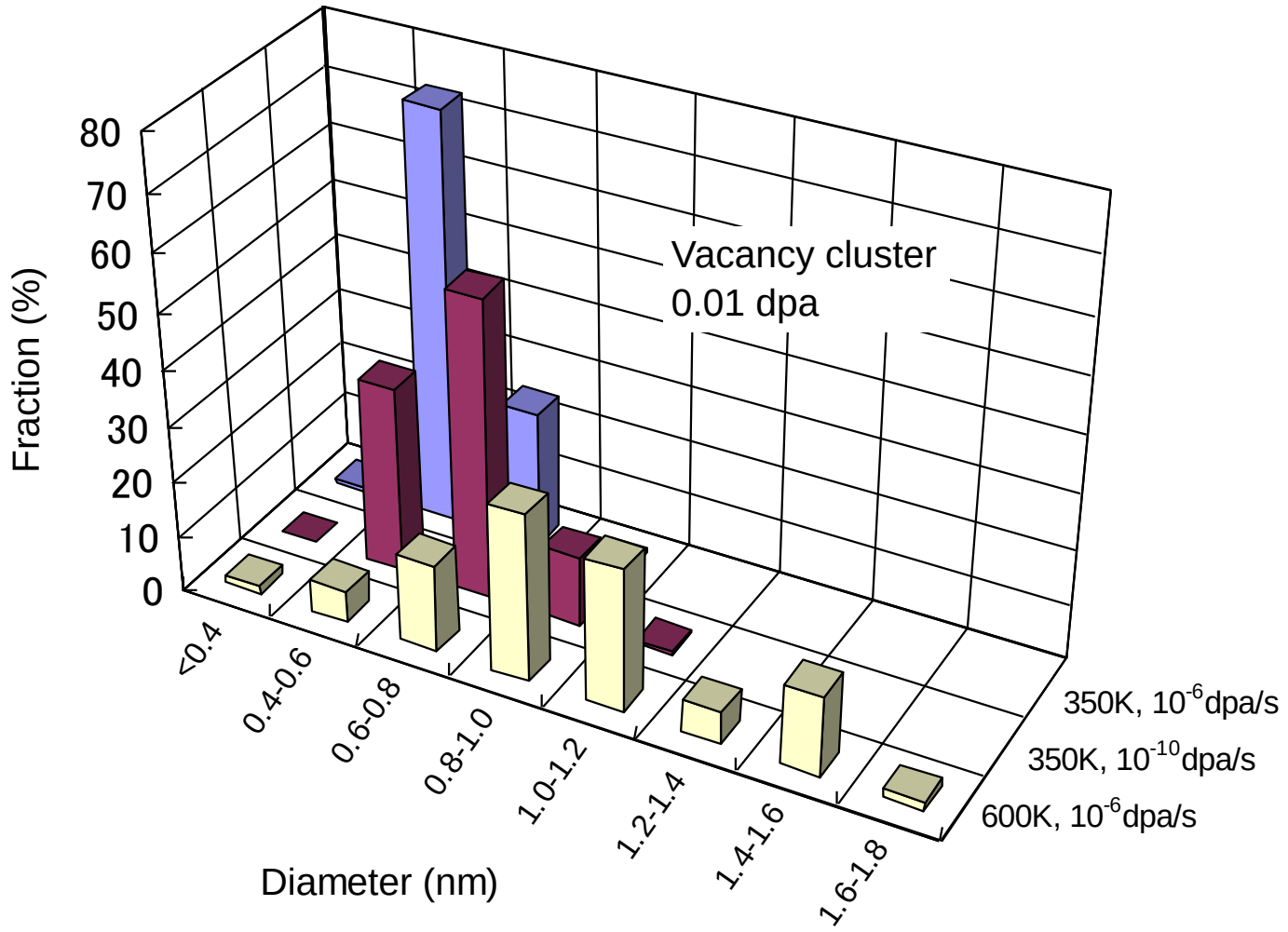




Vacancy clusters are unstable at low dose rates

SIA cluaters are stable at all the dose rates.

Temp. Effect on V Cluster Size



Temperature Effect in bcc-Fe

Experimental correlation

Jones & Williams

$$SMD = A \cdot F_T \cdot (\phi t)^{0.5}$$

$$F_T = 1.869 - 4.57 \times 10^{-3} T$$

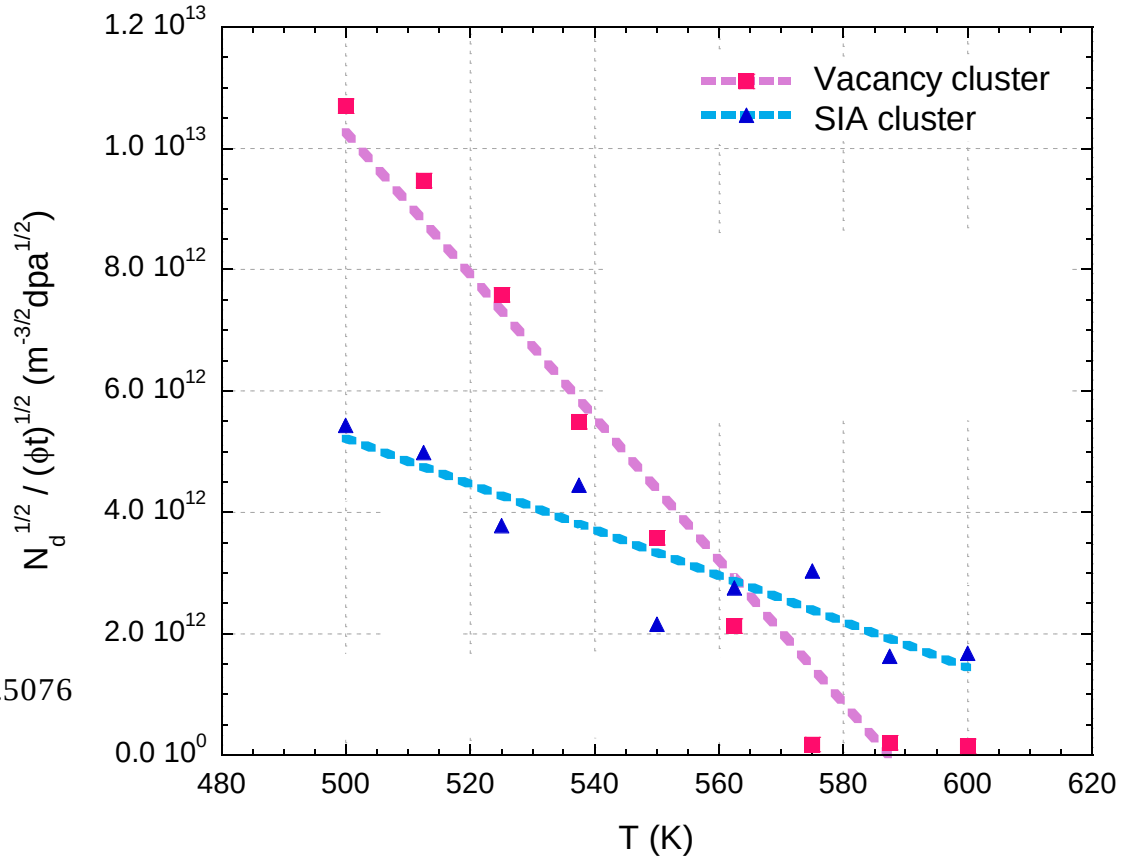
(T : 100 ~ 350°C)

ASTM E 900-02

$$SMD = A \cdot \exp\left(\frac{20{,}370}{T_c + 460}\right) \cdot f^{0.5076}$$

(T in °F)

Kinetic Monte Carlo Simulation

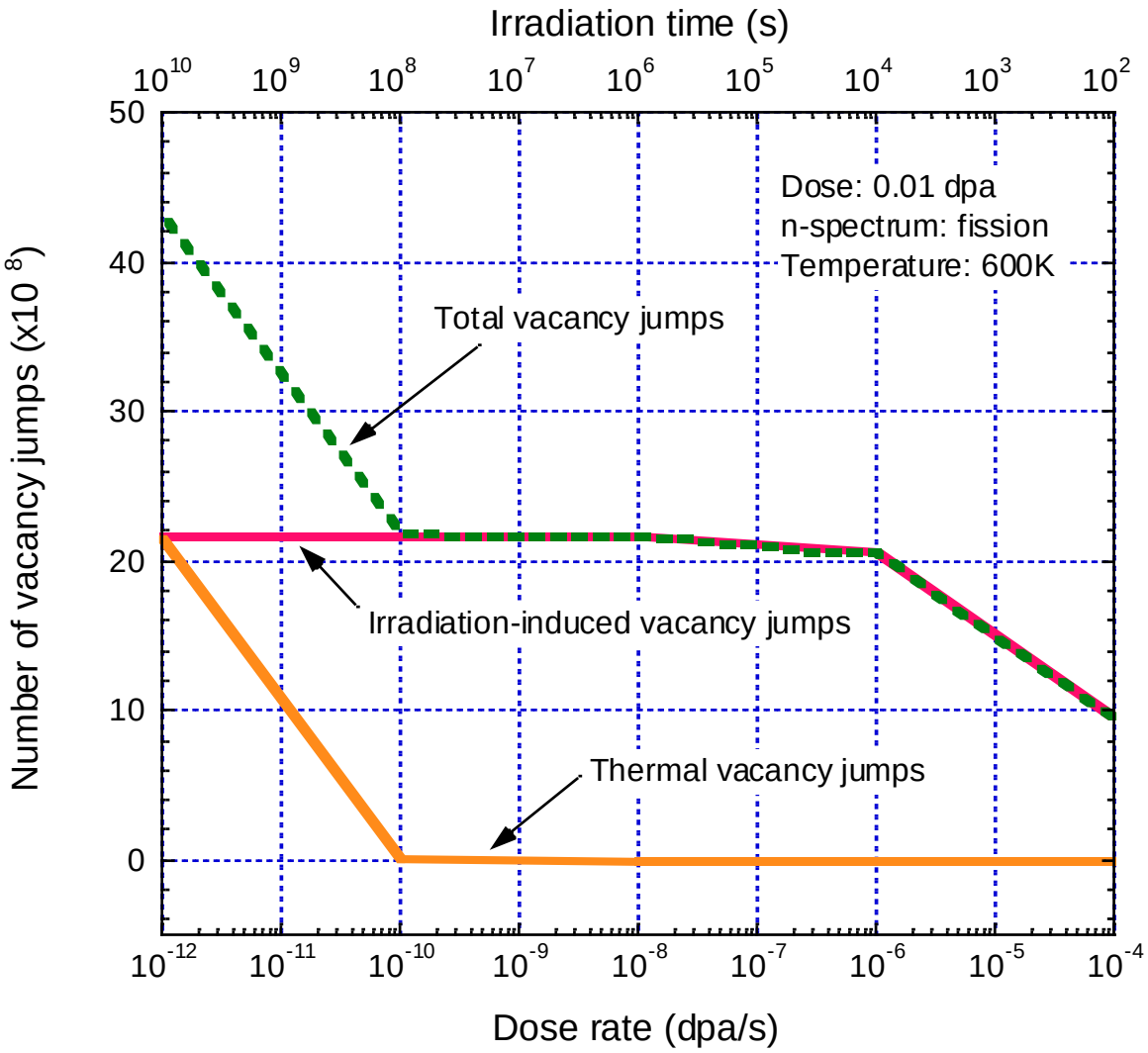


Estimation of the Number of Vacancy Jumps

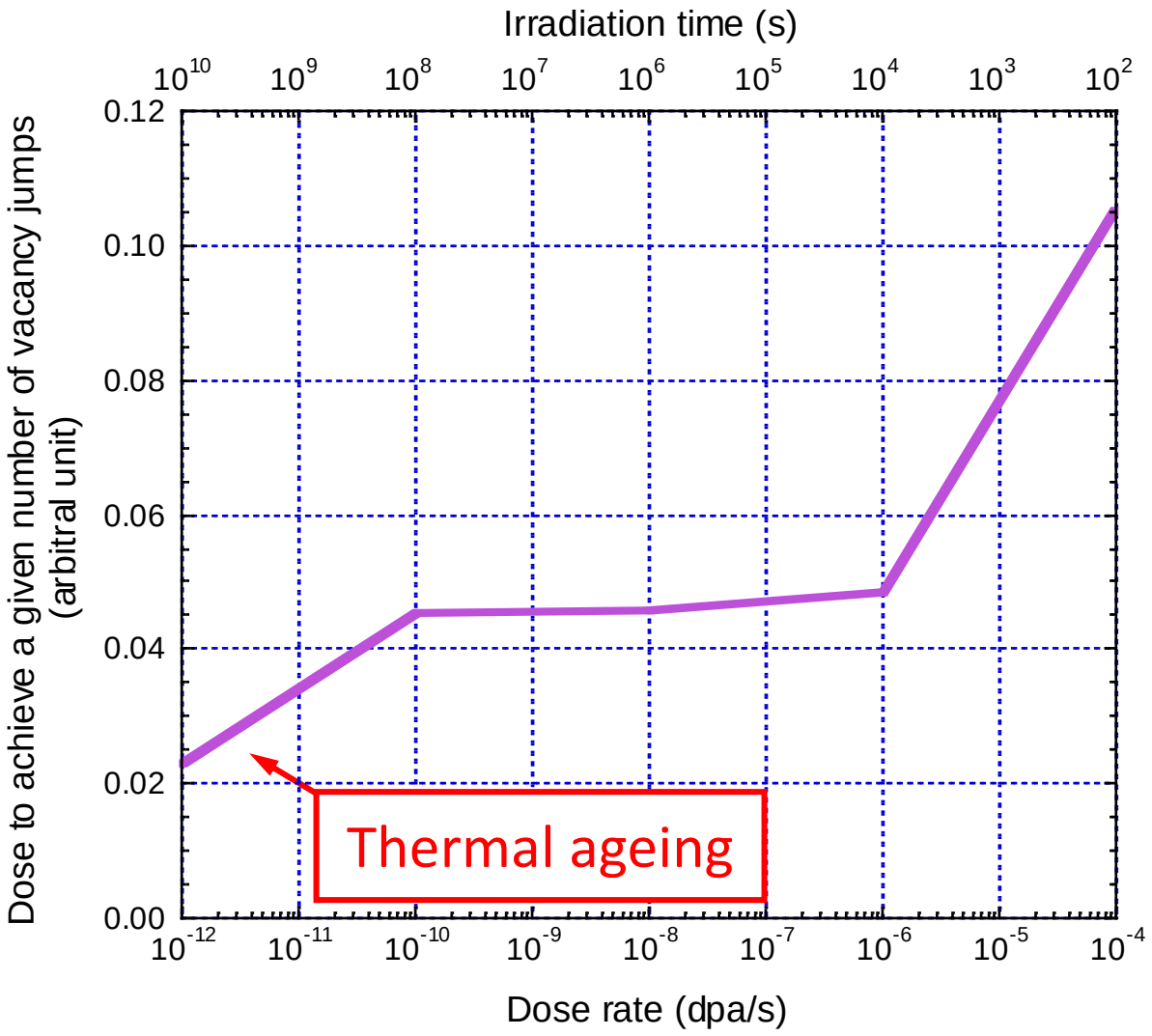
- Diffusion of vacancies leads to the diffusion of solute atoms such as copper.
- Effect of dose rate on the number of vacancy jumps can be a qualitative measure of the dose rate effect on the solute diffusion (and clustering).
- The number of thermal vacancy jumps can be estimated as:

$$n_{th} = t \cdot \frac{6}{\delta^2} \cdot D_0 \cdot \exp\left(-\frac{E_m^v}{kT}\right) \cdot 2\left(\frac{\ell}{a_0}\right)^3 \cdot \exp\left(\frac{S_k}{k}\right) \cdot \exp\left(-\frac{E_f^v}{kT}\right)$$

Effect of Dose Rate on the # of Vacancy Jumps



Doses Necessary to Achieve a Given # of V Jumps



Conclusions

- KMC simulations of defect accumulation in bcc-Fe during neutron irradiation were performed using the data set mostly obtained by MD simulations.
- Direct formation of large SIC clusters has some effects on the microstructural evolution.
- Effect of dose rate on the defect accumulation was studied.
  - There is a threshold dose rate below which no (or very small) flux effect is observed on the point defect clustering, maybe due to loss of cascade overlapping.
  - The contribution of thermal vacancies is not negligible at very low dose rates.