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

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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 range
- 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

Cumulative fraction of defects in clusters

Cluster size

SIA cluster (20keV)
Vacancy cluster (20keV)
SIA cluster (50keV)
Vacancy cluster (50keV)
Classification of defect formation again

50keV

- 53% Small* SIA clusters & small vacancy clusters
- 15% Large* SIA clusters & small vacancy clusters
- 5% Large SIA clusters & large vacancy clusters
- 17% Channeling**
- 10% Dispersed defect production**

- 73% (small cluster)
- 27% (large cluster)

20keV

- 80% Small* SIA clusters & small vacancy clusters
- 10% Large* SIA clusters & small vacancy clusters
- 8% Large SIA clusters & large vacancy clusters
- 2% Channeling**
- 10% Dispersed defect production**

- 90% (small cluster)
- 10% (large cluster)
Small SIA & small vacancy cluster

3.17 psec

Isolated subcascades

10.04 psec

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

Black dots : vacancies
White circles : SIAs

Case 45
Large SIA & small vacancy cluster

Overlapping of subcascades of similar sizes

Large SIAs are formed at the overlap region of the subcascades.

Black dots: vacancies
White circles: SIAs

Case 09
Overlapping of subcascades of different sizes

Case 28

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.
Large SIA & large vacancy cluster (2)

One large cascade, and then ...
Large SIA & large vacancy cluster (3)

Cascade collapse in α-Fe

Black dots: vacancies
White circles: SIAs

Case 39

40.02 psec
Channeling

<112> direction

- Black dots: vacancies
- White circles: SIAs

Periodic boundary condition

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

<table>
<thead>
<tr>
<th>Direction</th>
<th>50keV</th>
<th>20keV</th>
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<tbody>
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</tr>
<tr>
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</tr>
<tr>
<td>⟨001⟩</td>
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<td>0</td>
</tr>
</tbody>
</table>
Dispersed defect production

Black dots: vacancies
White circles: SIAs
Gray: replaced atoms
Case 42

Periodic boundary condition

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</tbody>
</table>

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

- Similar size distribution
- Peak sizes are similar
- Longer tail of distribution in 50keV

Size of the largest vacancy cluster in cascade

- 50keV cascade
- 20keV cascade
Structure of cascades – SIA –

- 50keV cascade has an additional peak at the size range of 11-14.
- Longer tail of distribution in 50keV
Structure of cascade

High energy

Small SIA cluster
(~5-8)

Medium SIA cluster
(~5-8 x 2 = ~10-16)

This may be the reason of additional peak in the SIA size distribution at the range of 11-14 in the side 16.

Large SIA cluster
(~100)

Large SIA cluster
(>100)

Small vacancy-rich zone
(3-8)

Large vacancy cluster
(>100)

: Unit structure
Cascade-overlap at high doses

4nm SIA loop + 50keV cascade

- pre-existing SIA loop
- cascade
- growth
- rotation
- No change
- dissociation

cascades
pre-existing SIA loop
pre-existing loop position
SIA loops
Cascade overlap statistics

- Growth: 63%
- Rotation: 21%
- Dissociation: 8%
- No change: 8%

(48 cases)
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).
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.

- 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

- Set event frequencies
- Accumulate frequencies
- Pick an event
- Update time
- Do the event

Repeat until a given time / dose is reached

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

- Diffusion $\rightarrow D_o, E_m$
- Dissociation $\rightarrow D_o, E_b+E_m$
- Cascade $\rightarrow$ dose rate

$$P = \sum_i N_i P_i$$

$$R = \text{Random()}*P$$

$$t = -\log(R) / P$$
Displacement Cascade Database of bcc-Fe

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

20keV (50 runs)

50keV (100 runs)

Small clusters

Channeling

Periodic boundary condition

Dispersed defect formation

Large SIA & V clusters

Large SIA clusters

Simulation of PKA Spectrum

Diffusion Kinetics of Point Defects in bcc-Fe

1D motion of SIA clusters

Rotation frequency model

Migration energy model

Binding Energies of Defect Clusters in bcc-Fe

Binding energy model

\[ E_b^I = 4.33 - 5.76(n^{2/3} - (n-1)^{2/3}) \quad \text{for} \quad n > 10 \]

\[ E_b^V = 1.73 - 2.59(n^{2/3} - (n-1)^{2/3}) \quad \text{for} \quad n > 8 \]
Finite Periodic Boundary Condition

Grain boundary

1\textsuperscript{st} cell

N\textsuperscript{th} cell

Computation cell

\begin{align*}
1\text{st cell} & : t = t_n \\
N\text{th cell} & : t = t_{n+1}
\end{align*}

\begin{itemize}
\item Particle that belongs to each home cell
\end{itemize}

Annihilation of particle A

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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 clusters are stable at all the dose rates.

Vacancy

SIA

Number density (m$^{-3}$)

Dose (dpa)

Temperature: 600K
n-spectrum: Fission
Grain size: 10µm

No stable vacancy cluster at $10^{-8}$dpa/s and $10^{-10}$dpa/s

SIA cluster > 37

$10^{-4}$ dpa/s

$10^{-6}$ dpa/s

$10^{-8}$ dpa/s

$10^{-10}$ dpa/s
Temp. Effect on V Cluster Size

Vacancy cluster
0.01 dpa

Diameter (nm)
Fraction (%)

350K, 10^{-6} dpa/s
350K, 10^{-10} dpa/s
600K, 10^{-6} dpa/s
Temperature Effect in bcc-Fe

Experimental correlation

Jones & Williams

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

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

\( (T : 100 \sim 350^\circ C) \)

ASTM E 900-02

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

\( (T \text{ in } ^\circ F) \)

Kinetic Monte Carlo Simulation

- Vacancy cluster
- SIA cluster
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

Dose: 0.01 dpa
n-spectrum: fission
Temperature: 600K
Doses Necessary to Achieve a Given # of V Jumps

Dose to achieve a given number of vacancy jumps

Irradiation time (s)

Dose rate (dpa/s)

Dose to achieve a given number of vacancy jumps (arbitrary unit)

Thermal ageing
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.