Object kinetic Monte Carlo for concentrated alloys

M. J. Caturla, M. J. Aliaga Dept. Física Aplicada, UA, Spain
L. Malerba, SCK-CEN, Belgium
A. Gokhman & F. Bergner HZDR, Germany

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Outline

- OKMC simulations of damage accumulation in FeCr: effective model and comparison to rate theory
- The source term for ion implantation experiments
- OKMC model for concentrated alloys
OKMC effective model for high Cr concentrations

- OKMC model for neutron irradiation of Fe12.5%Cr to compare with cluster dynamics (A. Gokhman, F. Bergner, et. Al [1])

- OKMC simulation set up:
  - 300nm x 300nm x 300nm simulation box
  - Single V, single I, clusters of size 2 and 4 for I, 2 and 6 for V
  - 140 ndpa/s

Simulation set up and parameters

Values considered after ref. [1]

- Vacancy formation energy = 1.6 eV
- Binding energy di-vacancy = 0.608 eV
- Vacancy migration energy = 0.88 eV
- Pre-factor vacancy migration = 2.1x10^{-8} (m^2/s)
- Self-interstitial formation energy = 3 eV
- Binding energy of di-interstitial = 0.8 eV
- Interstitial migration energy = 0.24 eV
- Pre-factor vacancy migration = 4x10^{-8} (m^2/s)

- Capture radius of 0.65 nm for single-vacancy and single-self-interstitial.
- Larger clusters considered as spheres with a geometrical radius depending on the number of defects.
- Bias for self-interstitials: 1.2 included in the capture radius.
- No sinks for defects (dislocations or grain boundaries) in the OKMC model.

Binding energies for larger clusters according to equation:

\[ E_{bni} = E_{fi} + \frac{E_{b2i} - E_{fi}}{2^{2/3}} \left[ n^{2/3} - (n-1)^{2/3} \right] \]
Average diameter of loops as obtained from OKMC compared to CD. Experimental results are also included [1]

Average radius of vacancy clusters from OKMC (blue line) and CD (red line)
Total number density of vacancy clusters for OKMC (blue line) and CD (red line)
Total number density of dislocation loops as a function of dose obtained from CD (red curve), OKMC (blue curve) and compared to TEM measurements
Includes also an OKMC simulation with sinks for single self-interstitials and single vacancies (green curve)
Removing the sinks from the CD calculations increases the total concentration but still far away from OKMC results.
Removing the sinks from the CD calculations does not change the average size of loops.
OKMC effective model: conclusions

• OKMC model reproduces interstitial loop sizes, vacancy loop sizes and vacancy concentrations but not self-interstitial concentrations

• Lack of sinks for self-interstitials in OKMC do not explain the discrepancies with CD for loops: capture volume (sphere vs. plane)?

  ➔ Importance of the initial defect size distribution
  ➔ Evolution of loops and vacancies together with Cr precipitation: how to include it in OKMC?
Molecular Dynamics simulations of cascade damage in bulk Fe: 50keV Fe in Fe

Carolina Björkas and Kai Nordlund

Large vacancy clusters are rarely observed in bulk cascades
Effect of free surfaces on cascade damage formation in Au
M. Ghaly, R. S. Averback & K. Nordlund

Dislocation structure

M. Ghaly and R. S. Averback,

Coherent displacement

Effect of free surfaces on cascade damage formation in Fe

Roger E. Stoller

Roger E. Stoller,
“The effect of free surfaces on cascade damage production in iron,”
Ion implantation in thin films for in situ TEM
Simulations setup

Number of atoms: 5 – 10 million
Energies: 50 – 500 keV
Temperature: approximately 0 K
Sample thickness: 40 – 80 nm
Calculations with MDCASK at Juelich HPC-FF supercomputer
Interatomic potentials: DD [1], AMS [2]

Ion implantation in thin films for in situ TEM
Cascade damage for 150keV and 500keV Fe in Fe
Anna Prokhodseva & R. Schaeublin (CRPP-EPFL), M. J. Aliaga(UA)

150 keV Fe collision in Fe thin film at 10°

40nm

100 keV Fe collision in Fe thin film at 22°

40nm

In some cases large damage is produced close to the surface.

In all cases the presence of the surface results in less self-interstitials than vacancies.

FeCr alloys, Edinburgh June 4-5, 2013
Ion implantation in thin films for in situ TEM
Cascade damage for 50keV Fe in Fe with AMS potential

50nm thickness

- 79% of all vacancies are in clusters
- 57% are in large clusters (>55 defects = 1nm loop)

- 98% of all interstitials in clusters
- 21% in large clusters

296 ad-atoms

Larger clustering of vacancies compared to bulk cascades
Ion implantation in thin films for in situ TEM
Cascade damage for 50keV Fe in Fe with AMS potential

83% of all vacancies are in clusters
67% are in large clusters
100% of all interstitials in clusters
0 in large clusters
312 ad-atoms

Larger clustering of vacancies compared to bulk cascades
Ion implantation in thin films for in situ TEM
Cascade damage for 50keV Fe in Fe with the AMS potential

50nm thickness

Interstitials
Vacancies
OKMC for concentrated alloys

- Need to model microstructure evolution in concentrated Fe-Cr alloys (2 - 20% Cr) under irradiation
- Need to go beyond rate theory due to large inhomogeneities in damage distribution
- OKMC models successful in modeling damage evolution in pure metals
- An explicit description of all alloy atoms would limit the system sizes that can be handled with OKMC
OKMC: methodology

**Input Data**

<table>
<thead>
<tr>
<th>Defect Distribution</th>
<th>From MD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rate for each Event</td>
<td>Defect Jump: Migration Energy</td>
</tr>
<tr>
<td></td>
<td>Cluster Dissolution: Binding Energy</td>
</tr>
<tr>
<td>R_i</td>
<td>New Cascade: Dose Rate</td>
</tr>
</tbody>
</table>

Until final time or dose

Total Rate, R: \( \sum R_i \times N_i \) with Ni number of particles for Event i

Select a particle from all the possible events: Random x R

Update Time: \( \text{Time} = -\log(\text{random})/R \)

Do Event: find neighbours of atoms that moved
1. The alloying element is not treated discretely but in terms of concentration.

<table>
<thead>
<tr>
<th>1 C₁</th>
<th>2 C₂</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>i Cᵢ</td>
<td>i+1 Cᵢ+₁</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td>...</td>
</tr>
</tbody>
</table>

2. Jump rates of particles are not fixed: will depend on the location of the particle and the environment.
Implementation steps

Step 1:
Cr represented in terms of average local concentration
OKMC simulation box divided into smaller boxes (cells) with different Cr concentration
Initial Cr distribution random in the simulation box
Two new input parameters in the simulation: Concentration of the alloy (in atomic %) and number of cells in each direction (x,y,z)

Example: Concentration of Cr in each cell
Simulation box size: 28nmx28nmx28nm
2x2x2 cells 4x4x4 cells
Implementation steps

Step 2:
Create defects at BCC lattice positions

Step 3:
Set jump probabilities for the defect depending on local Cr concentration and concentration of neighboring cells:

*Before:* Jump rate of a vacancy had a fixed value: $E_m^0 = 0.67 \text{eV}$

*Now:* Jump rate of a vacancy will depend on the local concentration, $c_1$, and the concentration of the neighboring cells, $c_2$.

Each vacancy will have associated different diffusion events
Each time a vacancy is created we have to look for neighboring positions that are in cells with different Cr concentration and account for those rates
The same process has to be done every time a vacancy jumps to a new location
Step 3:
Example:
A vacancy is created in cell 1 with alloy concentration $C_1$

- The location of all neighbors is determined (BCC lattice) and the type of neighbor
- The probability of that vacancy jumping to any of its nearest neighbors is evaluated depending on the location and type of the neighbors.

For example: the migration energy could be: $E_m^0 + w(c2-c1)$
Step 4:

After a vacancy jumps the concentration of the alloy or the matrix element in the original cell where the vacancy was located and the final cell where the vacancy jumped has to be evaluated.
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nm x 11.4nm x 11.4nm
Number of cells: 2
Temperature: 300K

Time = 0s

Time = 100s
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nm x 11.4nm x 11.4nm
Number of cells: 2
Temperature: 300K

Time = 500s

Time = 1000s
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nm x 11.4nm x 11.4nm
Number of cells: 2
Temperature: 300K

Time = 2000s
Other examples with larger number of cells

Example:

- Alloy concentration: 20%
- Vacancy concentration: 1 vacancy in the whole box
- Simulation box: 11.4nm x 11.4nm x 11.4nm
- Number of cells: 64 (4x4x4)
- Temperature: 300K

We start with an inhomogeneous distribution of Cr
Other examples with larger number of cells

Example:
Alloy concentration: 20%
Vacancy concentration: 1 vacancy in the whole box
Simulation box: 11.4nm x 11.4nm x 11.4nm
Number of cells: 64 (4x4x4)
Temperature: 300K

We start with an inhomogeneous distribution of Cr
Example 1 Precipitate (10%Cr) and 1% Cr in all other cells

Example:

- Alloy concentration: 1 atomic%
- Vacancy concentration:
  - 1 vacancy in the whole box

Simulation box: 11.4nm x 11.4nm x 11.4nm
- Number of cells: 64
- Temperature: 300K

Time = 0s
Example 1 Precipitate (10%Cr) and 1% Cr in all other cells

Example:
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nm x 11.4nm x 11.4nm
Number of cells: 64
Temperature: 300K
Conclusions and on-going work

• Comparison between CD and OKMC – good results except for total interstitial loop concentration – what is the difference between the two models?
• Damage close to surfaces significantly different from that at the bulk. In particular MD shows the formation of vacancy loops
• Taking into account the diffusion of alloy atoms and biasing the migration according to local concentrations we can model precipitation
• OKMC model must be improved to account for the correct behavior of precipitation and segregation of Cr at different temperatures and concentrations
Acknowledgements

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