Cascades by molecular dynamics in metals: interatomic potentials and BCA comparison, statistics

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ITEM Network

- European network
- EDF Coordinator
- 7 technical areas
- 40 members
- 4 years (starting 1/10/2001)
- Objectives:
  - to prepare new simulation tools by solving key problems and by giving some recommendations...
  - to build the European DAtabase for Multiscale modelling (EDAM)

Final report:

Guideline for Multi-scaling Modeling of Irradiation Effects

FIS5-2001-00031
Microstructure modeling evolution: Towards long irradiation

- Modelling complex chemistry + defects (point defects and clusters)
  - Atomic Kinetic Monte Carlo (AKMC) / OKMC / hybrid / rate theory
  - Data on defect solute clusters mobility & stability
  - Primary damage

- Primary damage
  - Prediction of empirical potentials
    - Representative
    - Quantitative
  - Threshold Displacement Energy
Multi-scale modelling

+ experimental validation

Finite elements

Code_ASTER

cm³

Micro-macro

μm³

Dislocation dynamics

Mesoscopic

MICROMEGAS

DFT

VASP

Molecular dynamics

DYMOKA

1nm³

0 - ps

(10-30nm)³

ns

Atomic & Object Kinetic Monte Carlo (30-100nm)³

h-year

s - h

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EAM Potential comparison

DYMOKA, NVE, PBC

[Graphs showing EAM potential comparison for FeCu I, FeCu II, and FeCu III, with histograms of cluster size (number of interstitials) and vacancies.]
BCA (Marlowe) – MD cross comparison

[Souidi JNM2001]
Microstructure evolution: importance of source term (OKMC)

[Souidi JNM2011]
Medium / long term microstructure evolution modelling

Kinetic Monte Carlo (KMC) simulation of irradiation

Atomic KMC

Object KMC

Cascades

PBC or surface

Frenkel pairs

Ageing (one single vacancy)

Box size \approx 30 - 100 \text{ nm}

V \approx 10^{-4} \mu\text{m}^3

t \approx h \text{ to yr (T, G dependent)}

\Gamma_X = \nu_X \exp\left(-\frac{Ea}{kT}\right)

[\text{JNM 335 (2004) 121–145}]

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Medium / long term microstructure evolution modelling

**KMC simulation of irradiation (n, ion)**

**Atomic** KMC
Rigid lattice cohesive model based on DFT calculations

**Object** KMC

Hybrid AKMC / OKMC

[Domain JNM 2018]

Hybrid AKMC / OKMC

[JNM 2004]

solute –

\(<111>\) SIA loop

DFT

[Domain JNM 2018]

\[D_n^{\text{FeMn}} = D_n^{\text{Fe}} e^{\beta \Delta F_n}\]

\[\Delta F_n \approx -K_n E_{b1}\]

\[K_n = m_l x_{Mn}\]

[Chiappetto NIMB 2015]

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TDE from first principles

**TDE simulation characteristics:**
- Non-cubic supercells: 504 atoms (6x6x7 bcc cells)
- Born-Oppenheimer MD: electronic convergence for each MD step
- Time step: 2 – 3 fs
- TDE energy discretisation: 1 eV
- On 2048 cores (IBM BlueGene Q) and 1024 cores (Cray XE6)
- need up to ~2 ps simulated time
- very, very core-hour expensive!!!

**Standard minimal potentials**
- \( \text{Fe}_{sd} = \text{Ar}4s^13d^7 \)

**and the semi-core potentials**
- \( \text{Fe}_{psd} = \text{Mg}3p^64s^13d^7 \)

<table>
<thead>
<tr>
<th>( E_f ) (eV)</th>
<th>( \text{Fe}_{sd} )</th>
<th>( \text{Fe}_{psd} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Config</td>
<td>250</td>
<td>250</td>
</tr>
<tr>
<td>Vac</td>
<td>2.16</td>
<td>2.16</td>
</tr>
<tr>
<td>( \langle 110 \rangle )</td>
<td>4.05</td>
<td>3.97</td>
</tr>
<tr>
<td>( \langle 111 \rangle )</td>
<td>4.79</td>
<td>4.64</td>
</tr>
<tr>
<td>( \langle 100 \rangle )</td>
<td>5.18</td>
<td>5.02</td>
</tr>
<tr>
<td>( \langle 110 \rangle - \langle 111 \rangle )</td>
<td>0.74</td>
<td>0.67</td>
</tr>
<tr>
<td>FP</td>
<td>6.21</td>
<td>6.05</td>
</tr>
</tbody>
</table>

[Olsson MRL2016]
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TDE angular anisotropy in Fe

- Very good agreement with experiments in high-symmetry directions
- About 5 eV difference between Fe_{sd} and Fe_{psd}

Average TDE:

\[ E_{d,\text{ave}}^{\text{av}} = \frac{\int_0^{2\pi} \int_0^\pi E^1_d(\theta, \phi) \sin \theta \, d\theta \, d\phi}{\int_0^{2\pi} \int_0^\pi \sin \theta \, d\theta \, d\phi} \]

- Fe_{sd}: 29 eV
- Fe_{psd}: 32 eV
- ASTM: 40 eV
- AM04: 39 eV

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TDE angular anisotropy in Fe

Very similar topology for $\text{Fe}_{sd}$ and $\text{Fe}_{psd}$

Not so similar to EAM (nor the analytical model of Seeger)

$\langle 110 \rangle$ is hyperbolic in DFT, minimal in EAM and maximal in Seeger

$\langle 111 \rangle$ is strongly maximal in EAM

[Olsson MRL 2016]
Drag atoms

Quasi-static drag simulations show difference between methods

One atom is dragged through the lattice and the energetic response is recorded without relaxation

ZBL, AM04 and Fe_{psd} are more or less in agreement (equally stiff) for the close packed directions

Fe_{sd} is much softer

[Olsson MRL 2016]
Drag atoms: isosurface

Isosurface 18 eV

\[ \text{Fe}_{\text{psd}} \quad \text{Fe}_{\text{sd}} \]

Isosurface 25 eV

\[ \text{Fe}_{\text{psd}} \quad \text{EAM (AM04)} \]
Density Functional Theory: Dynamic simulation of defect creation

- DFT simulation of 40 eV knock-on in <100> direction
- BO-DFT

Static Calculations:

W

[JNM 470 (2016) 116]

(a) Displacement in the (111) direction. (b) Displacement in the (101) direction.

[Sand JNM2016]
TDE & Quasi Static Drag (QSD) correlation

MA10B2
MA10A
CO21013N
CO21013D
CO21620
CO30912
MEND10

Reduced units

CO2 & CO3: Marinica et al.

〈100〉

〈110〉
BCA (SDTrimSP) – MD cross comparison
Sub-cascades analysis

1 MeV PKA in W

[De Backer EPL2016]
Defect size distribution

MD cascades – DYMOKA code – <135> & random PKA
PBC – constant volume
Very large statistics
Around 500 – 1000 cascades / PKA energy / potential / T
PKA energy: 1 keV to 160 keV  (@ 100K)

For PKA >=80 keV
- 50% mono defects
- 10% SIA clusters > 100

Pot Fe: EAM Ackland 2004

[Domain to be published]
Sub cascades
BCA (SDTrimSP) – MD cross comparison

[De Backer to be published]

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Fe [Ackland 04] – 80 keV PKA
Fe [Ackland 04] – 80 keV PKA
Transition metals comparison (Zr, Fe, Ni, W)

E_PKA = 50 keV

Defect size distribution

[Domain to be published]

[De Backer to be published]
Conclusions

- Large cascade database
  - Defect size distribution (PKA energy, potentials)
  - Good comparison and complementarity with BCA
  - Effect of potentials: equilibrium & hardening
    - Assessment / hardening of potentials based on DFT
    - Some Similarities for other metals (e.g. Zr, Ni, W, Mo)
  - Impact on microstructure modelling
    - Different class of objects formed (e.g. loops)
- Database
  - Potential: tabulated (no functions)
  - All atomic positions (XYZ format)
- Experimental validation
  - TEM invisible defects: HDS, ...
  - Low temperature controlled irradiation, isochronal annealing
  - Modelling of experiments (e.g. TEM, HDS, PA)