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

[1] Cluster Dynamics Study of Neutron Irradiation Induced Defects in Fe-12.5at%Cr Alloy, A. Gokhman, A. Ulbricht, U. Birkenheuer, F. Bergner, Solid State Phenomena 172-174 *(2011) 449*

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 = 2.1×10^{-8} (m^2/s)

Self-interstitial formation energy = 3 eV

Binding energy of di-interstitial = 0.8 eV

Interstitial migration energy = 0.24 eV

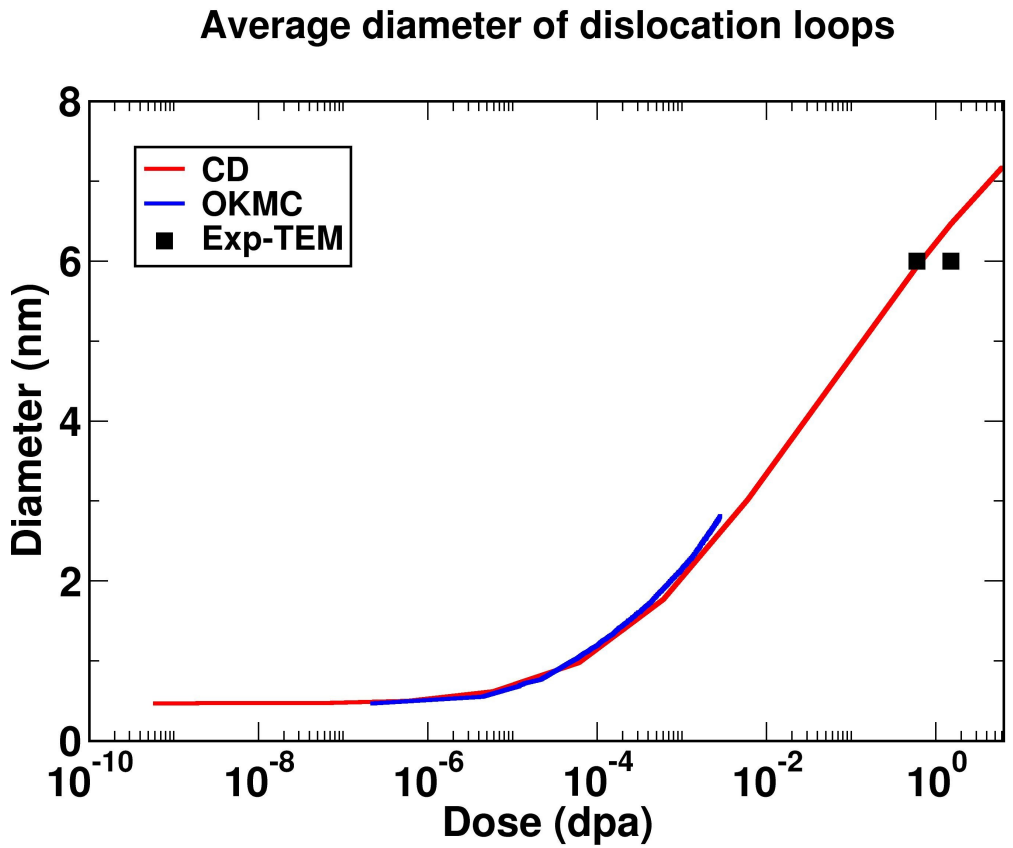
Pre-factor vacancy migration = 4×10^{-8} (m^2/s)

- 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:

$$E_{bni} = E_{fi} + \frac{E_{b2i} - E_{fi}}{2^{2/3} - 1}\left[n^{2/3} - (n-1)^{2/3}\right]$$

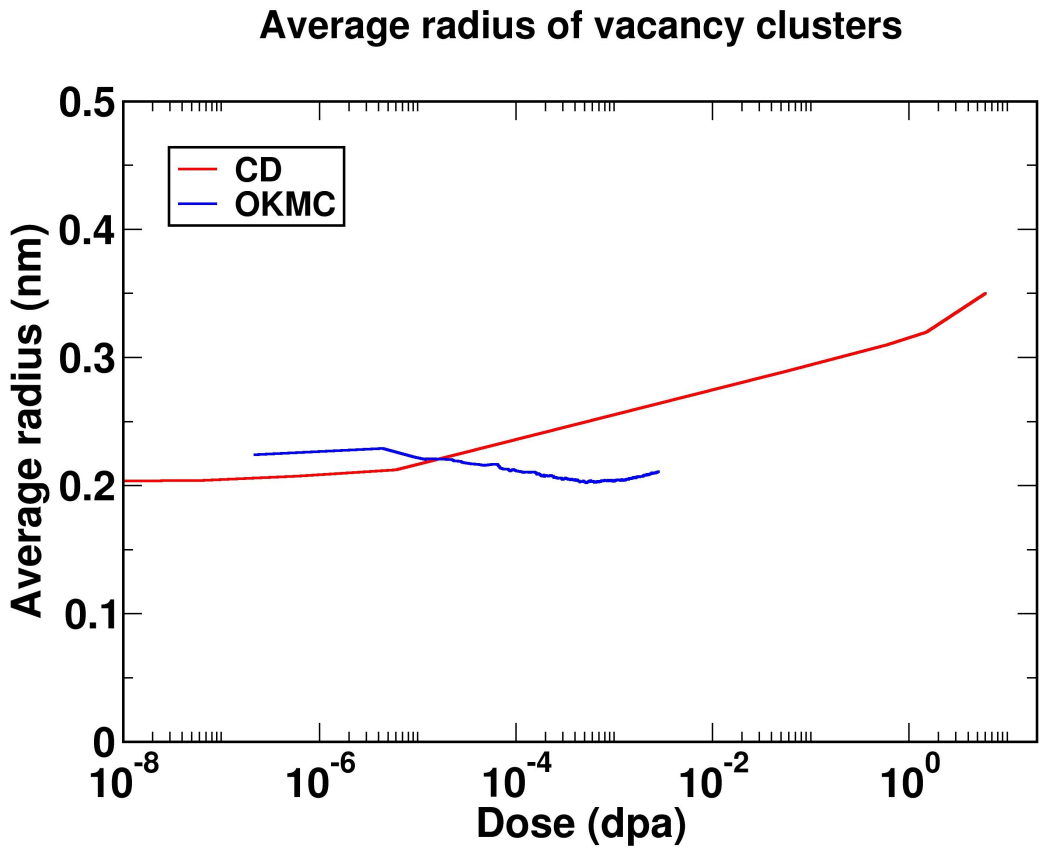
OKMC effective model



Average diameter of loops as obtained from OKMC compared to CD. Experimental results are also included [1]

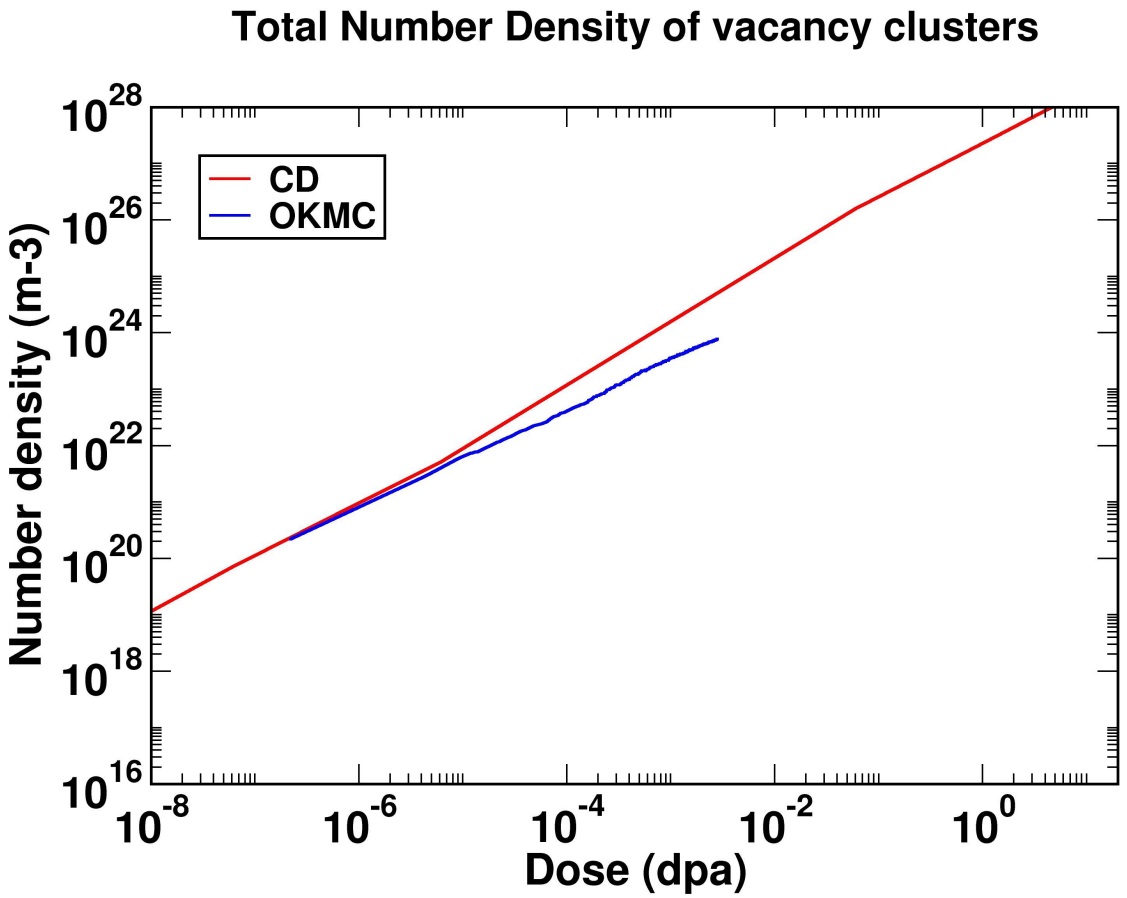
[1] Cluster Dynamics Study of Neutron Irradiation Induced Defects in Fe-12.5at%Cr Alloy, A. Gokhman, A. Ulbricht, U. Birkenheuer, F. Bergner, Solid State Phenomena 172-174 (2011) 449

OKMC effective model



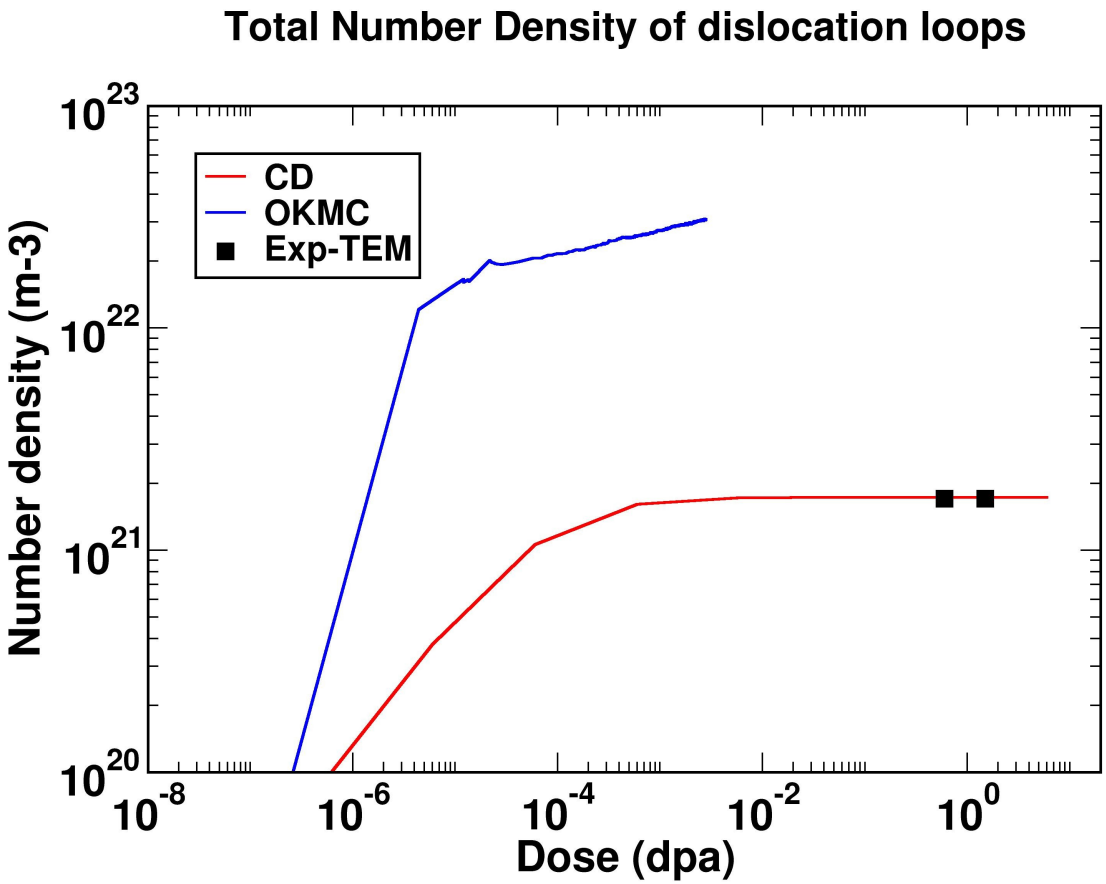
Average radius of vacancy clusters from OKMC (blue line) and CD (red line)

OKMC effective model



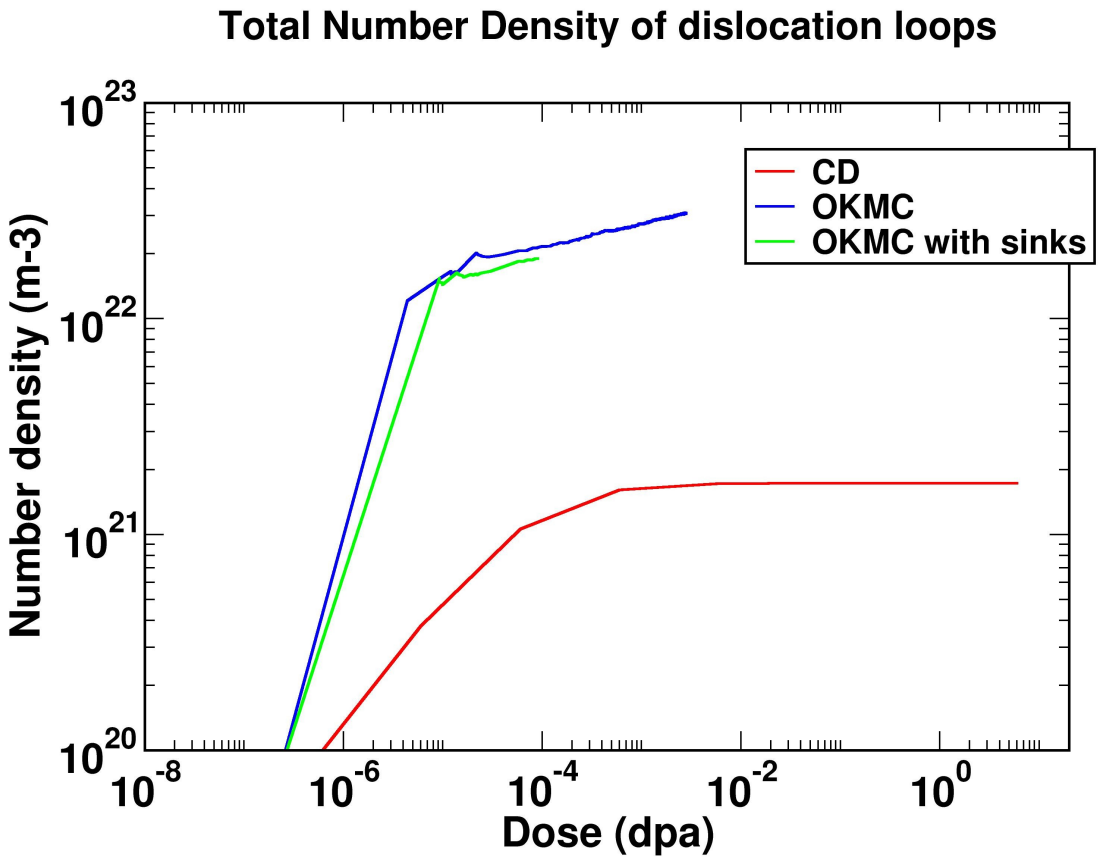
Total number density of vacancy clusters for OKMC (blue line) and CD (red line)

OKMC effective model



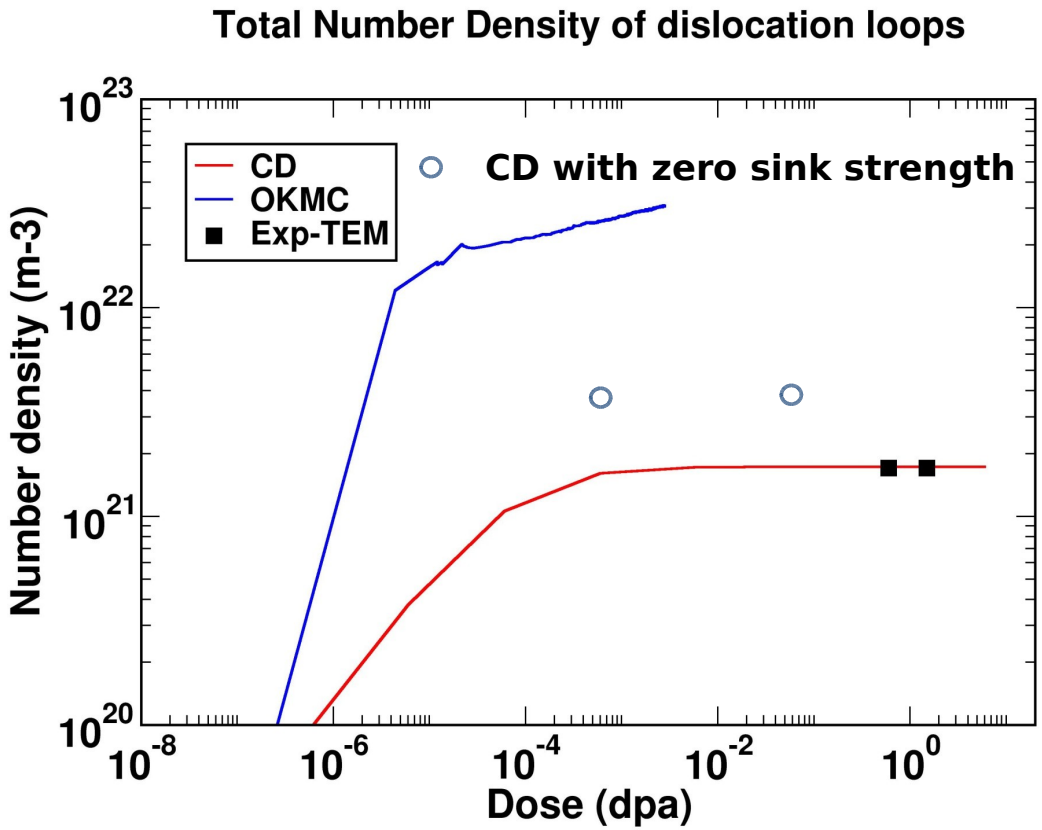
Total number density of dislocation loops as a function of dose obtained from CD (red curve), OKMC (blue curve) and compared to TEM measurements

OKMC effective model



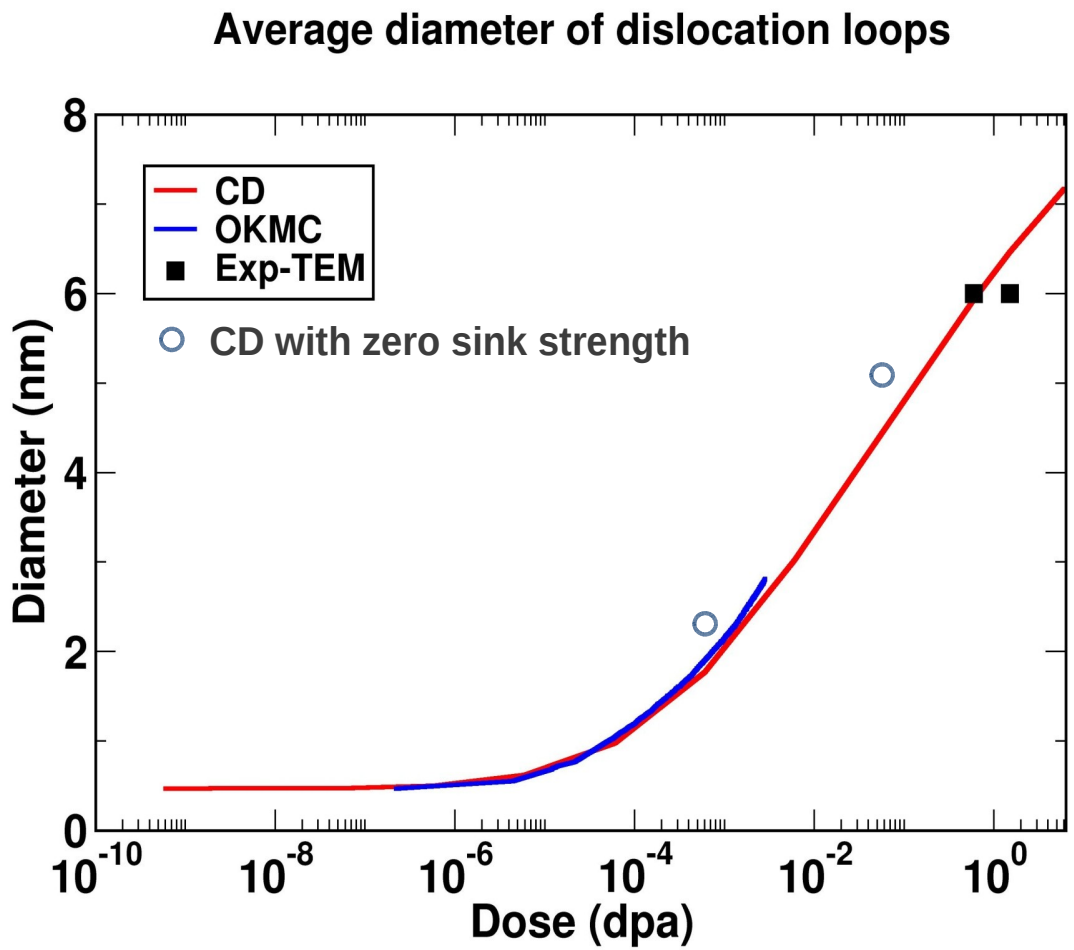
Includes also an OKMC simulation with sinks for single self-interstitials and single vacancies (green curve)

OKMC effective model



Removing the sinks from the CD calculations increases the total concentration but still far away from OKMC results

OKMC effective model



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) ?

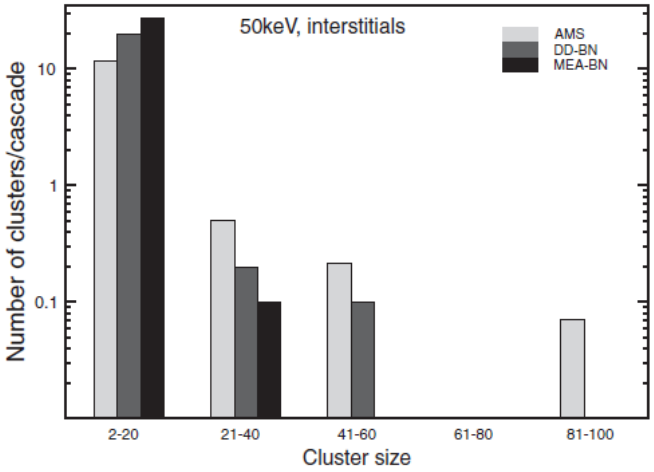
→ *Importance of the initial defect size distribution*

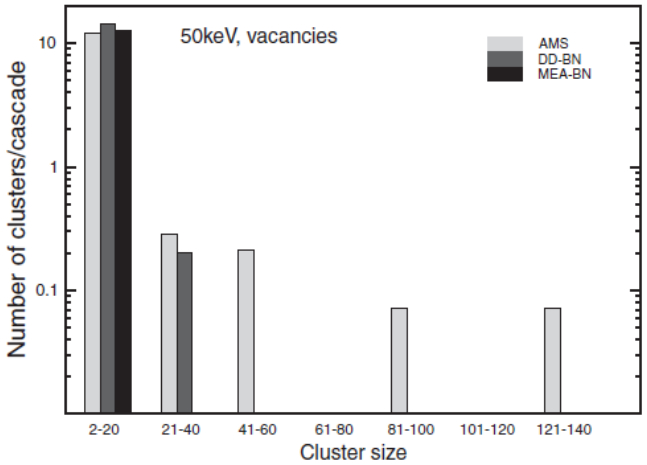
→ *Evolution of loops and vacancies together with Cr precipitation: how to include it in OKMC?*

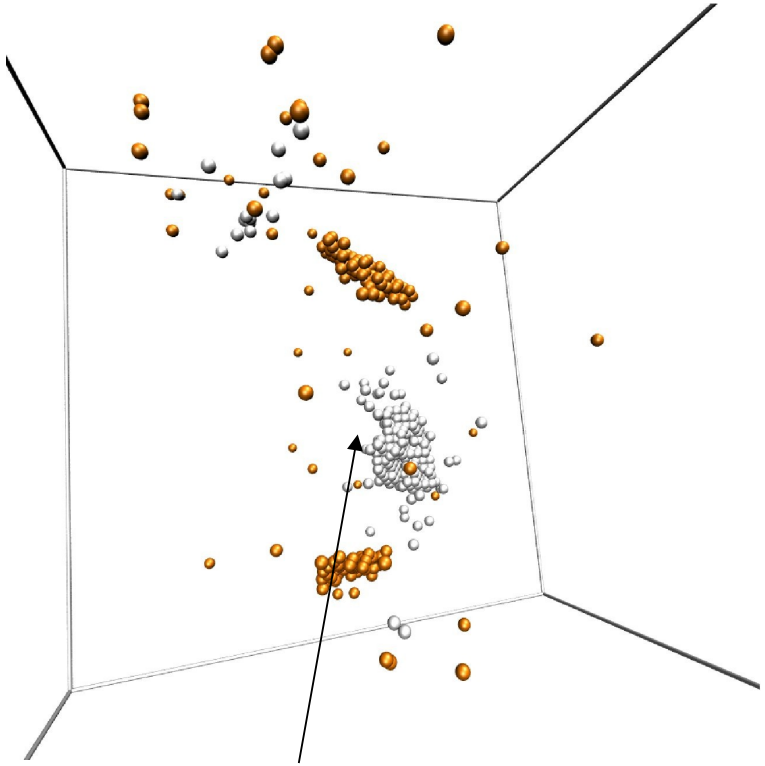
Molecular Dynamics simulations of cascade damage in bulk Fe: 50keV Fe in Fe

Carolina Björkas and Kai Nordlund

Nucl. Instrum. And Meth.B 267, 1830 (2009)
Phys. Rev. B 85, 024105 (2012)



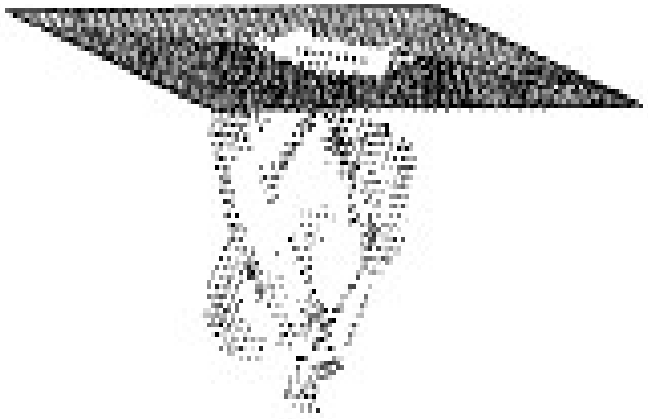




Large vacancy clusters are rarely observed in bulk cascades

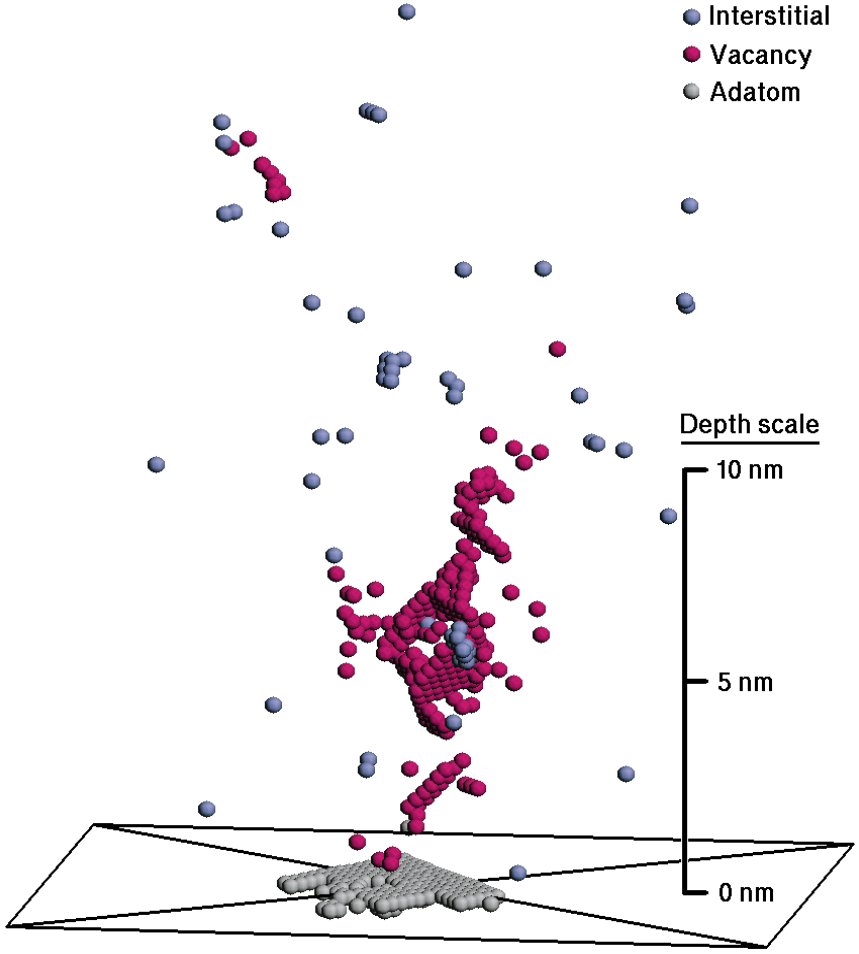
Effect of free surfaces on cascade damage formation in Au

M. Ghaly, R. S. Averback & K. Nordlund



Dislocation structure

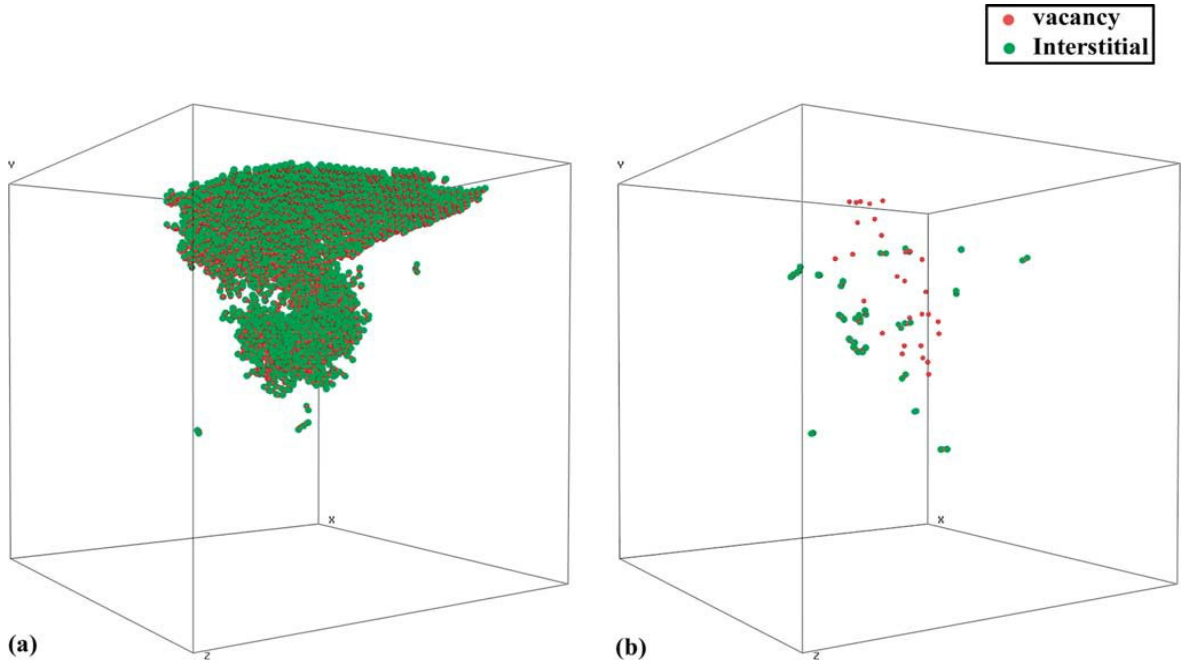
M. Ghaly and R. S. Averback,
"Effect of Viscous Flow on Ion Damage
near Solid Surfaces," Phys. Rev. Let. 72, 1994.



Coherent displacement

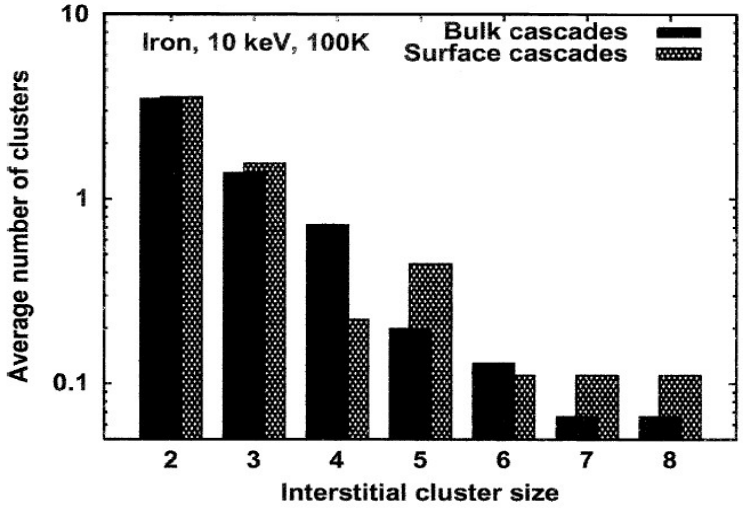
K. Nordlund et al., "Coherent displacement of atoms during ion irradiation", Nature 398, 1999

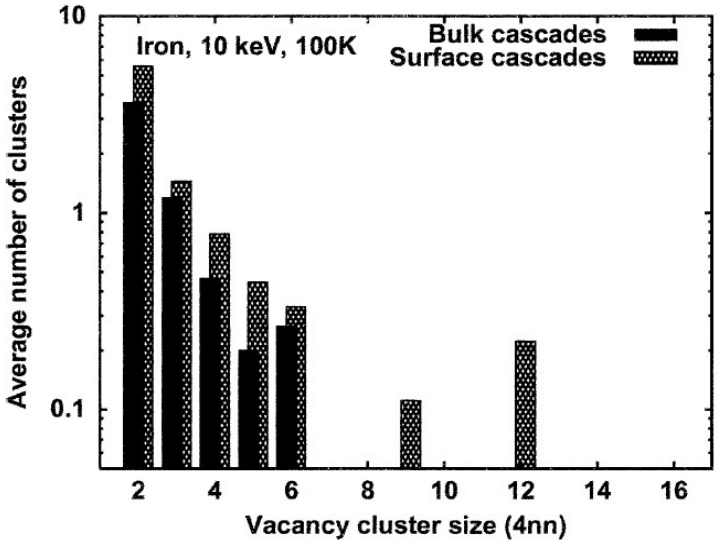
Effect of free surfaces on cascade damage formation in Fe
Roger E. Stoller



10keV Fe in Fe

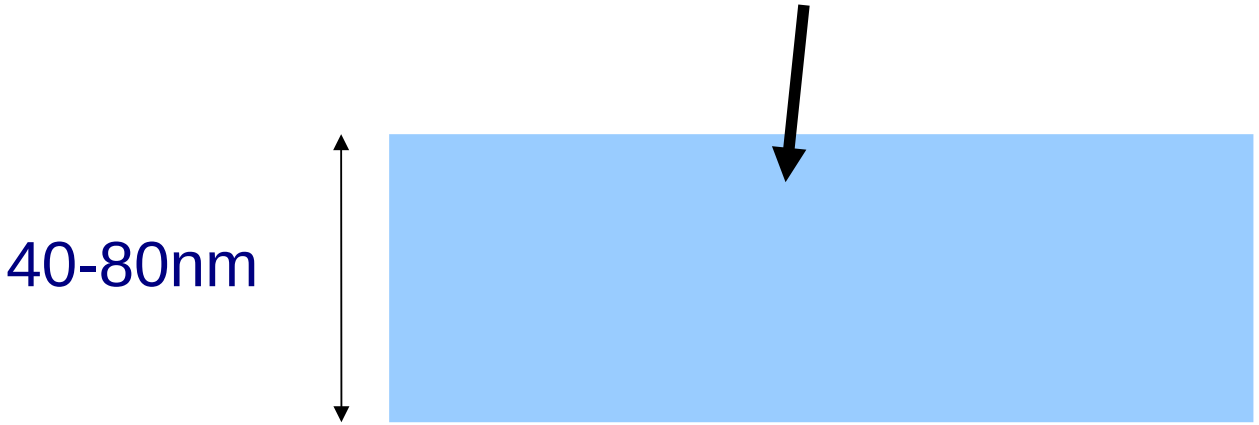
Roger E. Stoller,
"The effect of free surfaces on cascade damage production in iron,"
J. Nucl. Mater. 307, 2002.





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]



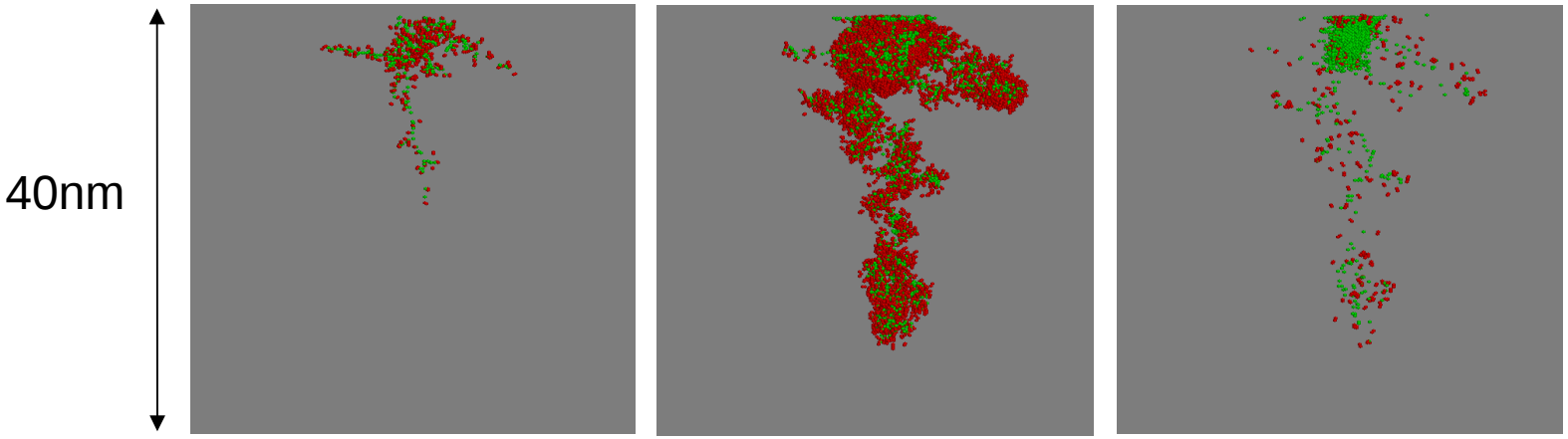
[1] S. L. Dudarev and P. M. Derlet. J. Phys.: Condens. Matter, 17 (2005).

[2] G. Ackland, M. I. Mendelev, D. J. Srolovitz, S. Han, A. V. Barashev, J. Phys: Condens. Matter. 16 (2004) S2629-42.

Ion implantation in thin films for in situ TEM
Cascade damage for 150keV and 500keV Fe in Fe

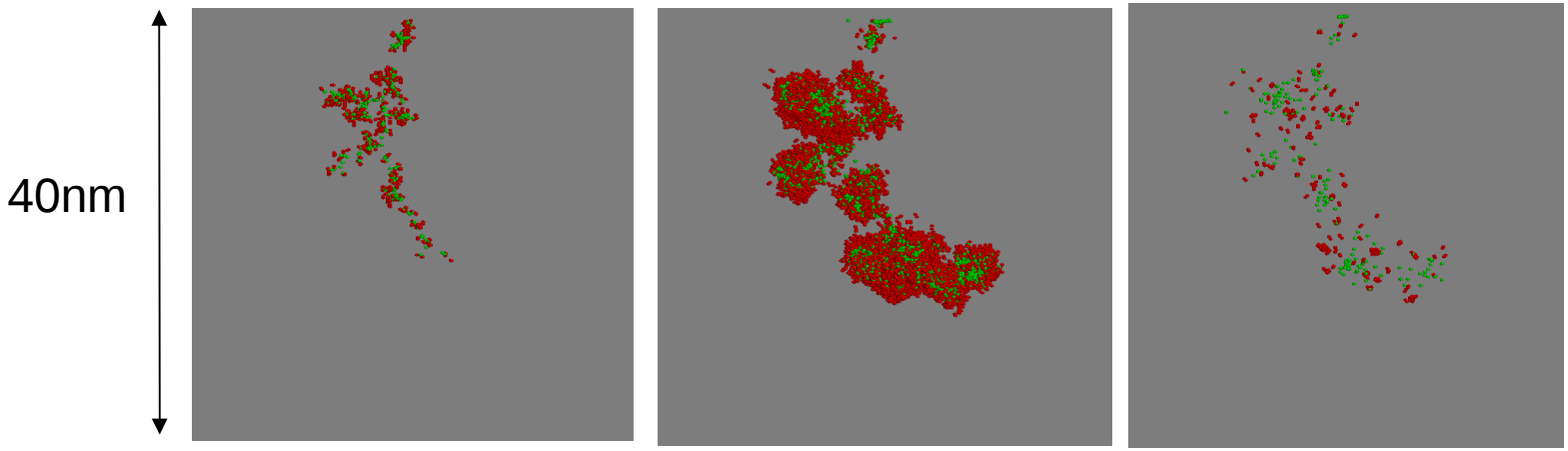
Anna Prokhodseva & R. Schaeublin (CRPP-EPFL), M. J. Aliaga(UA)

150 keV Fe collision in Fe thin film at 10°



In some cases large damage is produced close to the surface

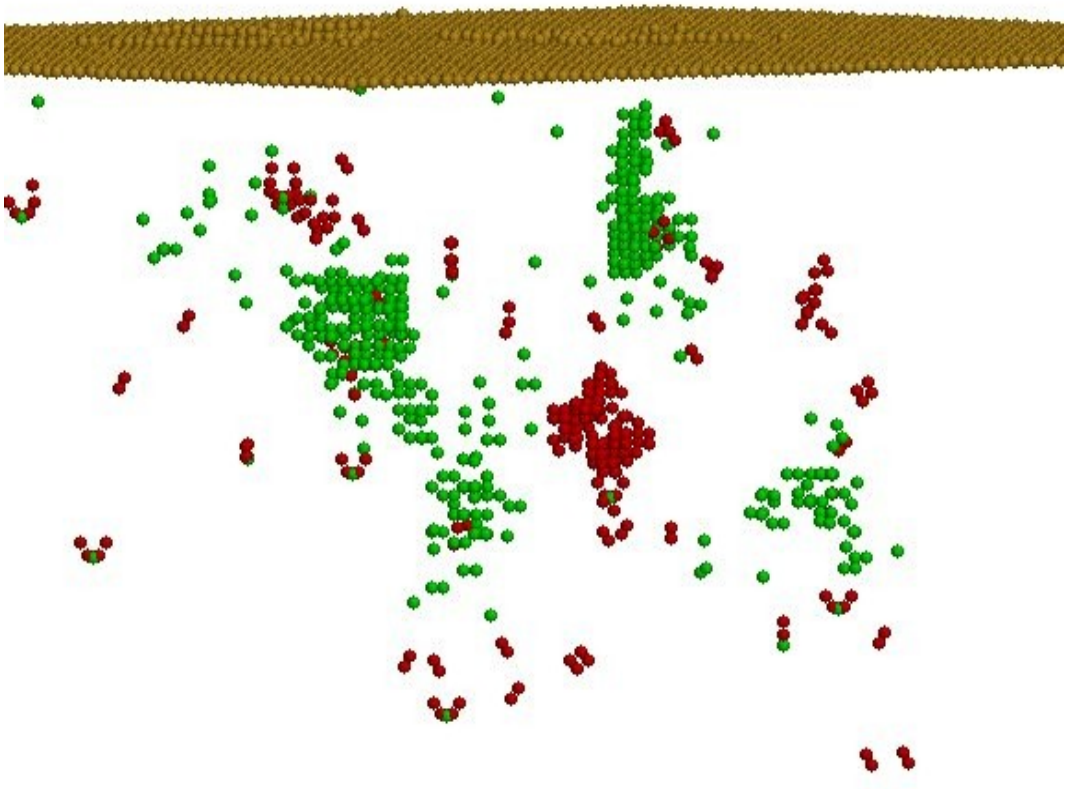
100 keV Fe collision in Fe thin film at 22°



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

Ion implantation in thin films for in situ TEM
Cascade damage for 50keV Fe in Fe with AMS potential

50nm thickness



- Interstitials
- Vacancies

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

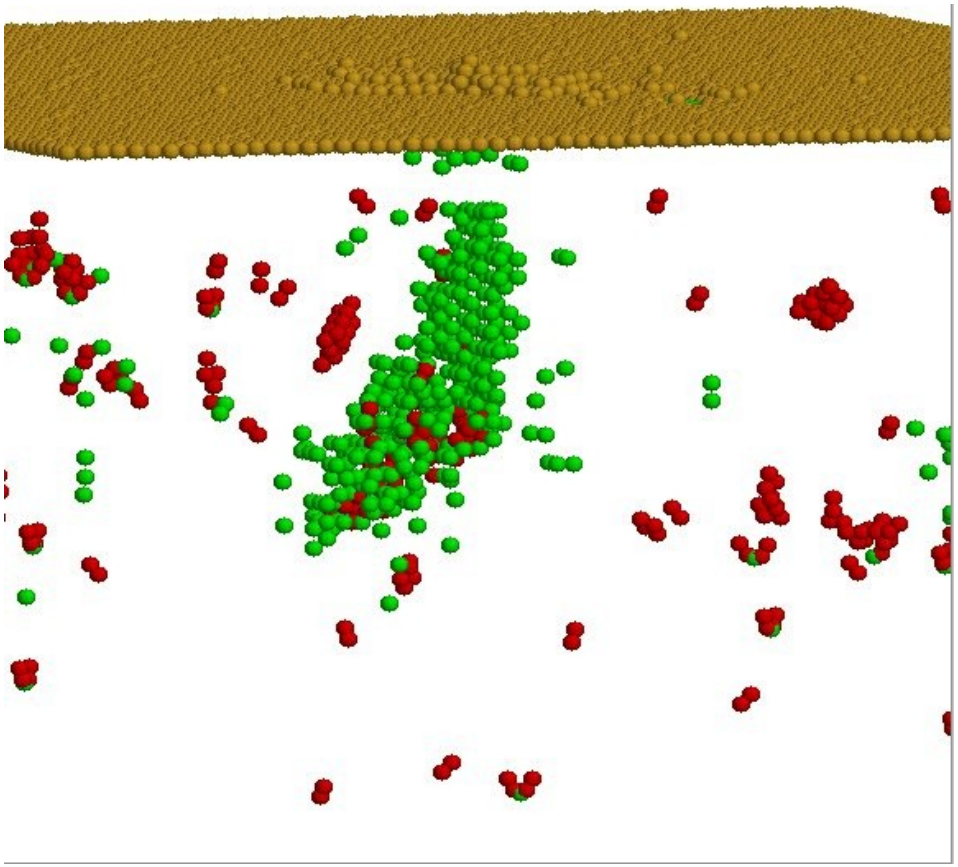
98% of all interstitials in clusters
21% in large clusters

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

50nm thickness



- Interstitials
- Vacancies

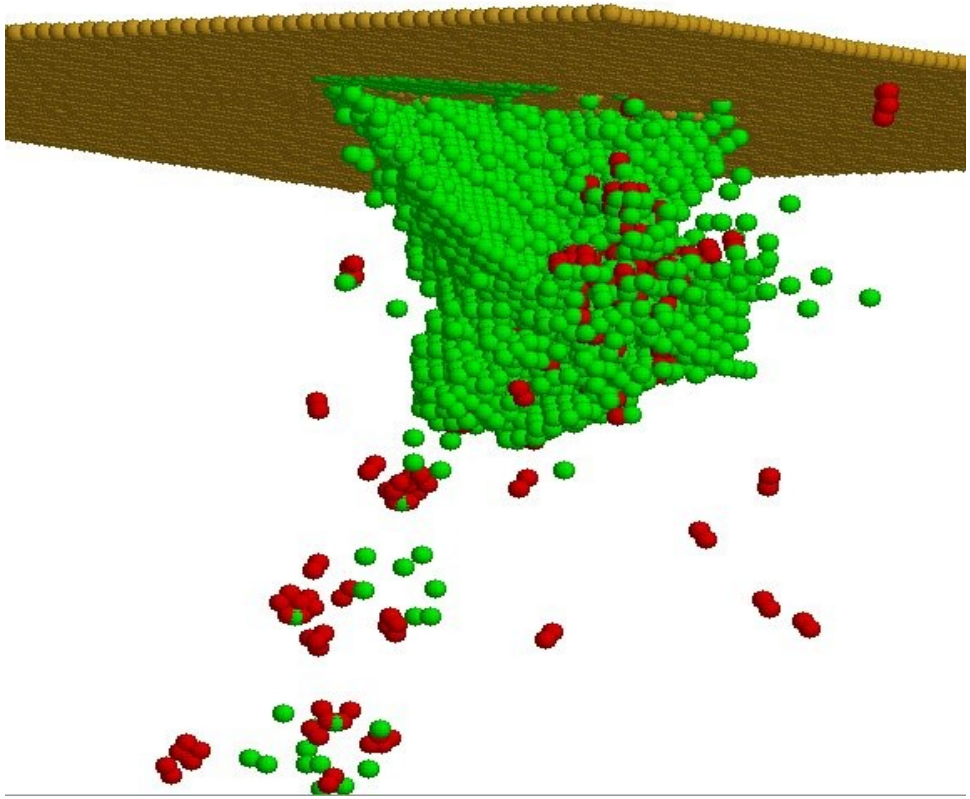
83% of all vacancies are in clusters
67% are in large clusters

100% of all interstitials in clusters
0 in large clusters

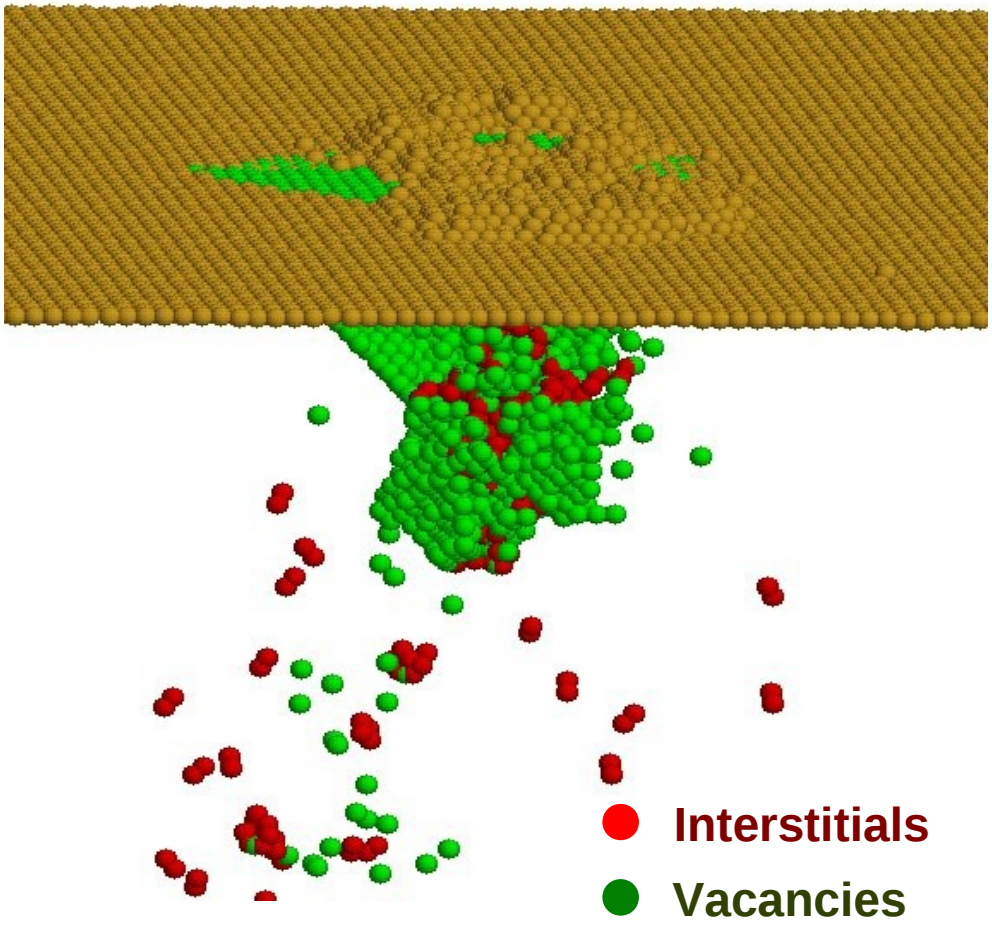
312 ad-atoms

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



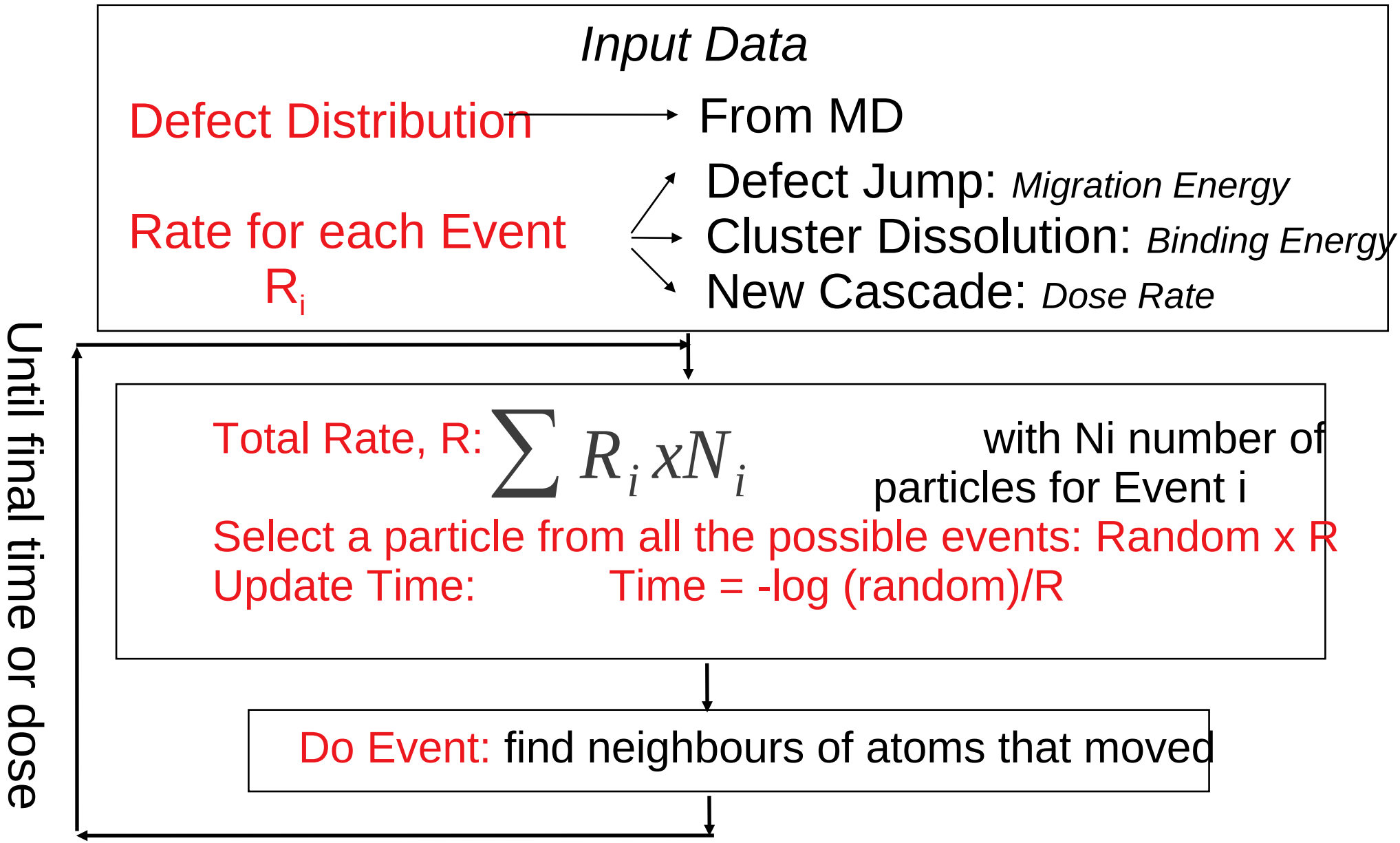
50nm thickness



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



OKMC model for concentrated FeCr alloys

1. The alloying element is not treated discretely but in terms of concentration

1 C_1	**2 C_2**	**…**
…	i C_i	i+1 C_{i+1}
	…	N C_N

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

Implementation steps

Step 1:

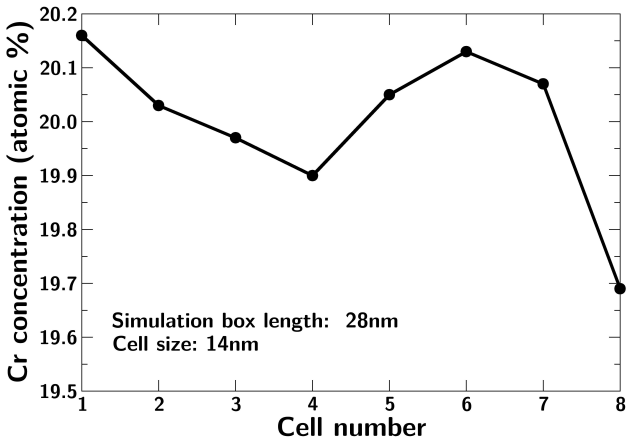
C_1	C_2	…
…	C_i	C_{i+1}
	…	C_N

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)

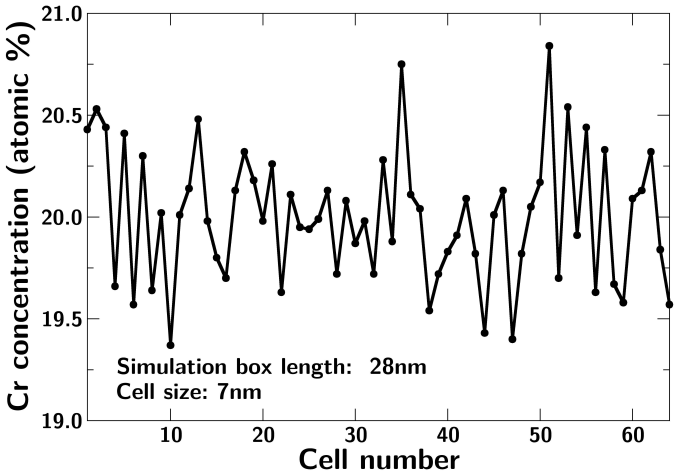
Example: Concentration of Cr in each cell

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: $E_m^0 = 0.67eV$

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

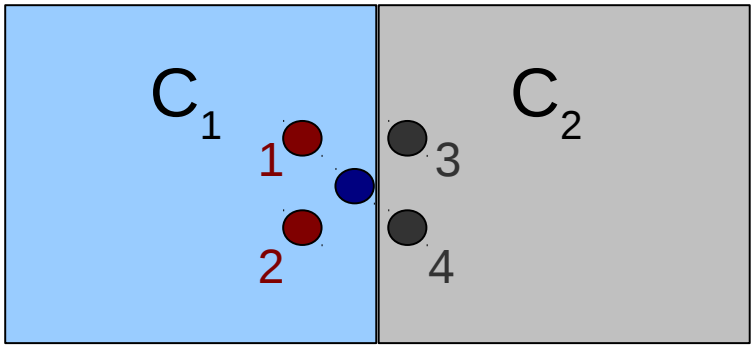
The same process has to be done every time a vacancy jumps to a new location

Implementation steps

Step 3:

Example:

A vacancy is created in cell 1 with alloy concentration C_1



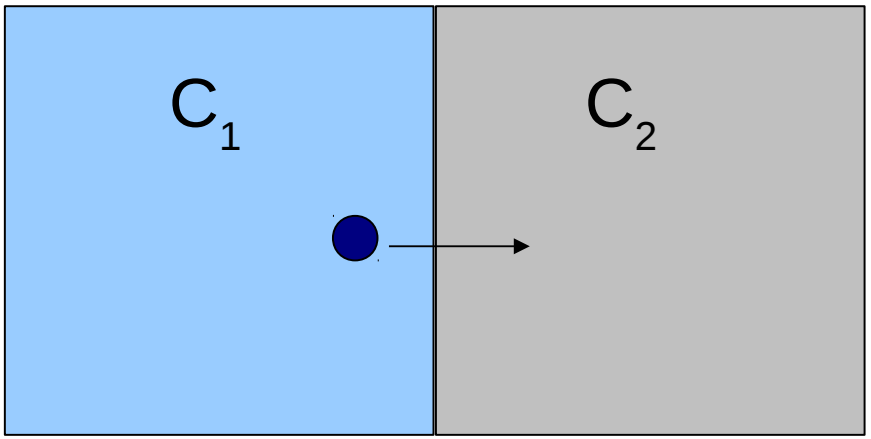
- The location of all neighbors is determined (BCC lattice) and the type of neighbor
- The probability of that vacancy jumping to any of its nearest neighbors is evaluated depending on the location and type of the neighbors.

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

Implementation steps

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



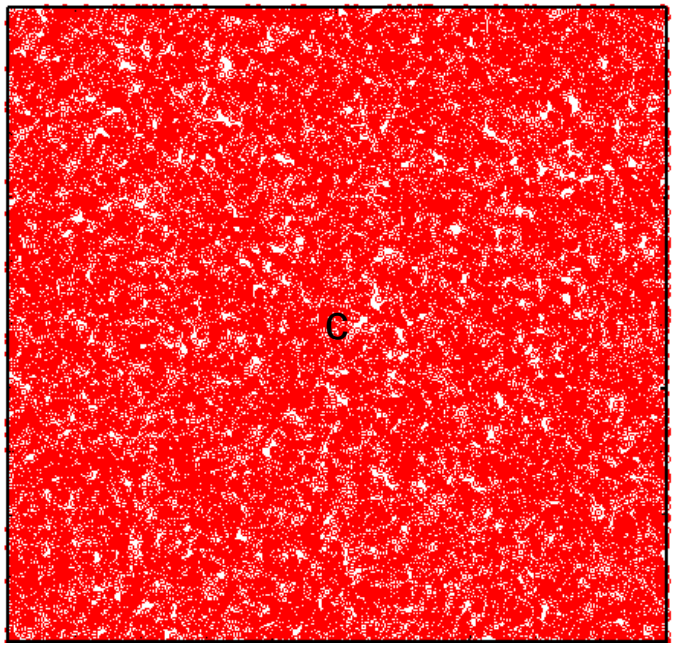
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:

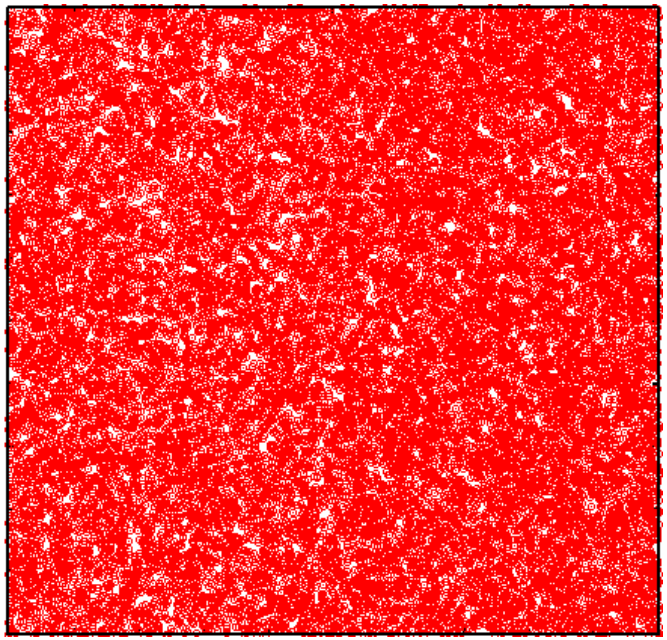
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nmx11.4nmx11.4nm
Number of cells: 2
Temperature: 300K

Time = 0s



Time = 100s



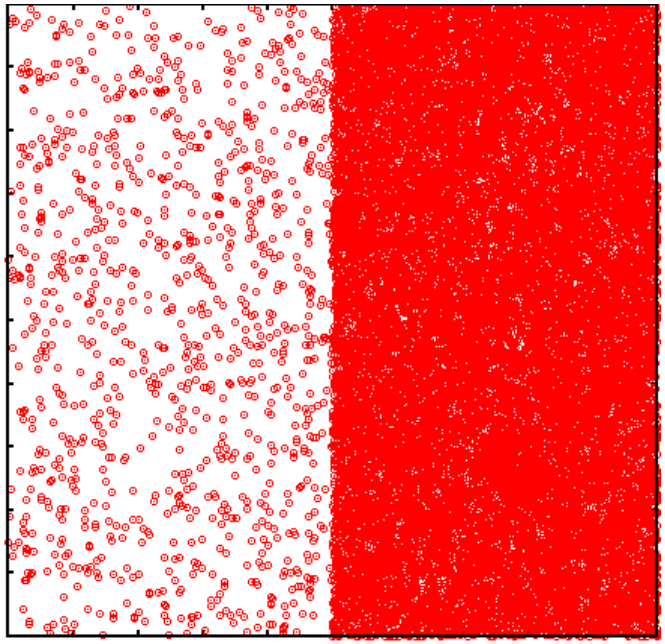
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:

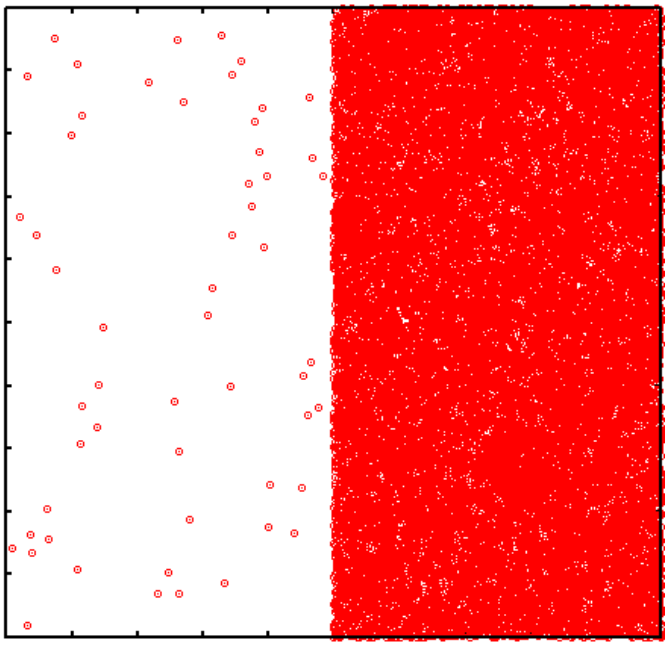
Alloy concentration: 1 atomic%
Vacancy concentration:
1 vacancy in the whole box

Simulation box: 11.4nmx11.4nmx11.4nm
Number of cells: 2
Temperature: 300K

Time = 500s



Time = 1000s



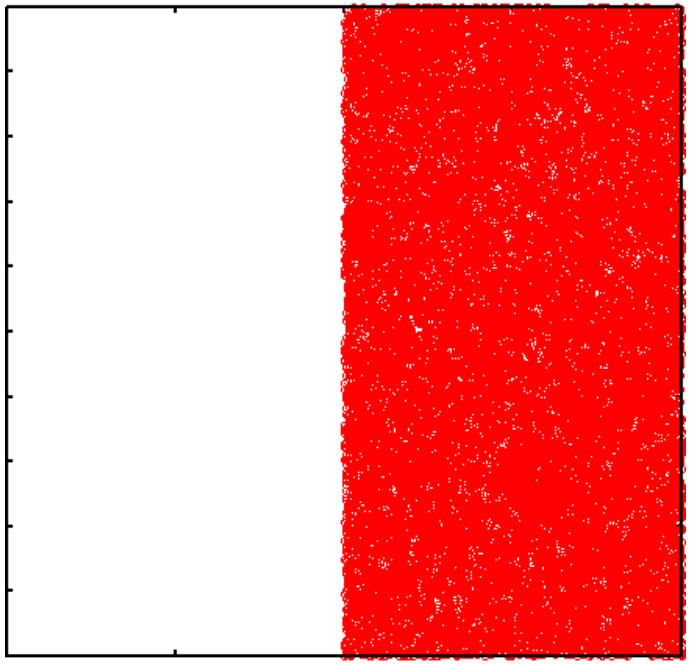
Example 2 cells at 20% Cr concentration
Evolution of Cr concentration in cells

Example:

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

Simulation box: 11.4nmx11.4nmx11.4nm
Number of cells: 2
Temperature: 300K

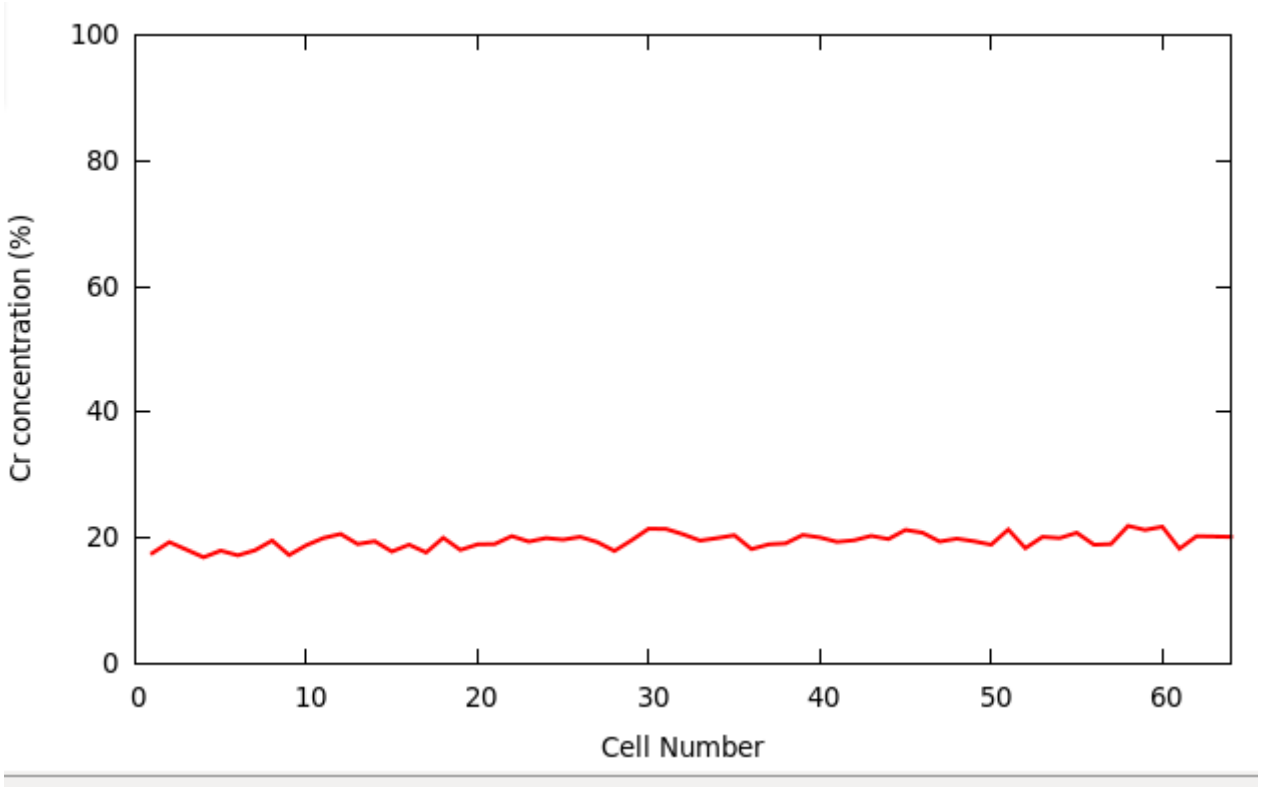
Time = 2000s



Other examples with larger number of cells

Example:

Alloy concentration: 20%
Vacancy concentration:
1 vacancy in the whole box
Simulation box:
11.4nmx11.4nmx11.4nm
Number of cells: 64 (4x4x4)
Temperature: 300K



We start with an inhomogeneous distribution of Cr

Other examples with larger number of cells

Example:

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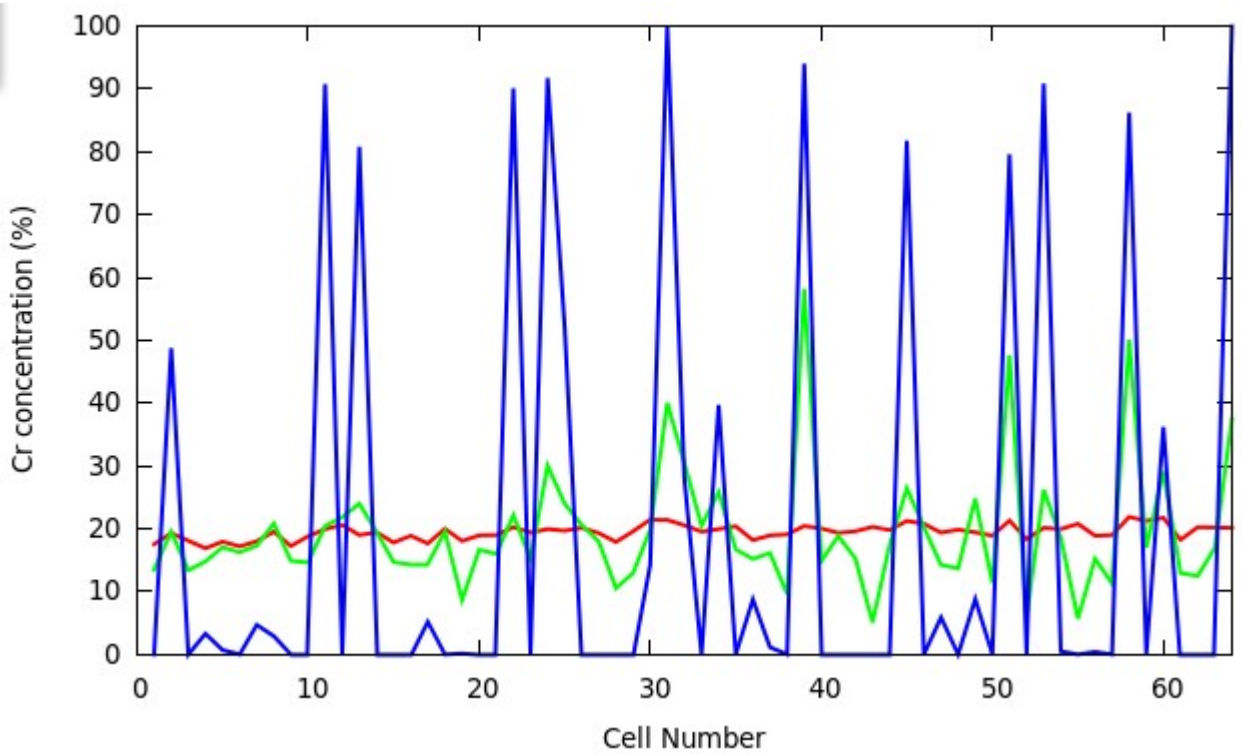
1 vacancy in the whole box
Simulation box:
11.4nmx11.4nmx11.4nm
Number of cells: 64 (4x4x4)
Temperature: 300K



We start with an inhomogeneous distribution of Cr

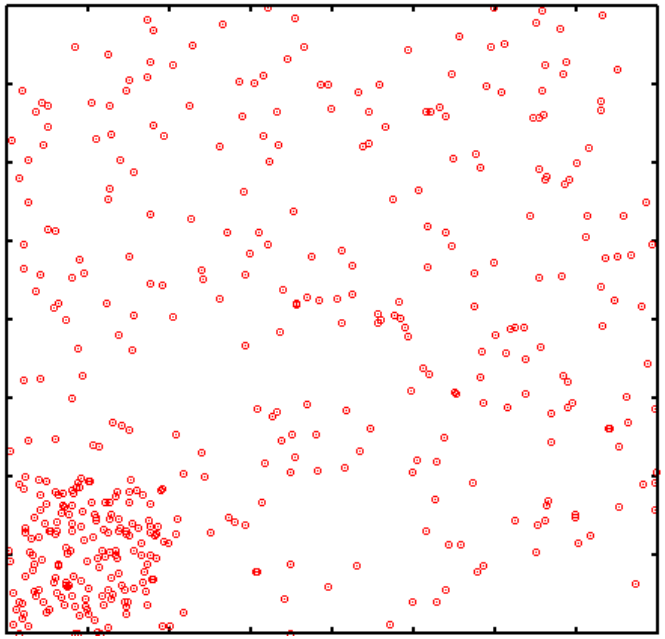
Example 1 Precipitate (10%Cr) and 1% Cr in all other cells

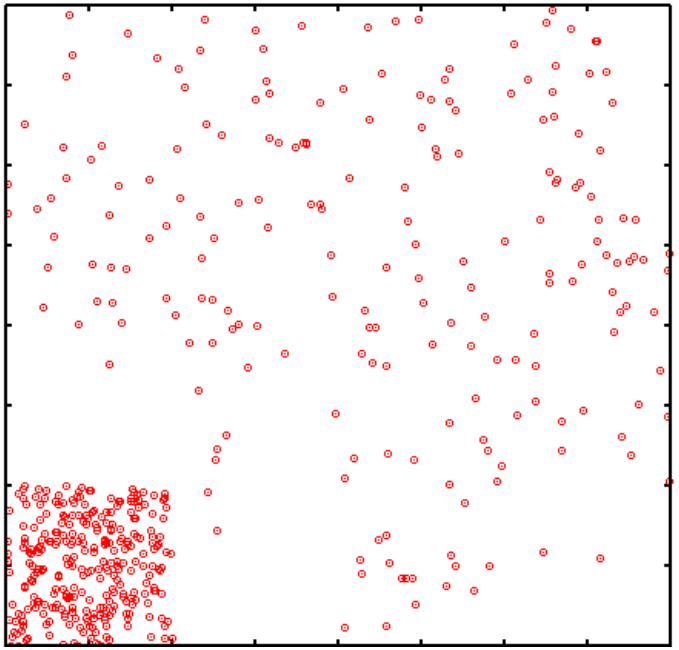
Example:

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

Simulation box: 11.4nmx11.4nmx11.4nm
Number of cells: 64
Temperature: 300K

Time = 0s





Example 1 Precipitate (10%Cr) and 1% Cr in all other cells

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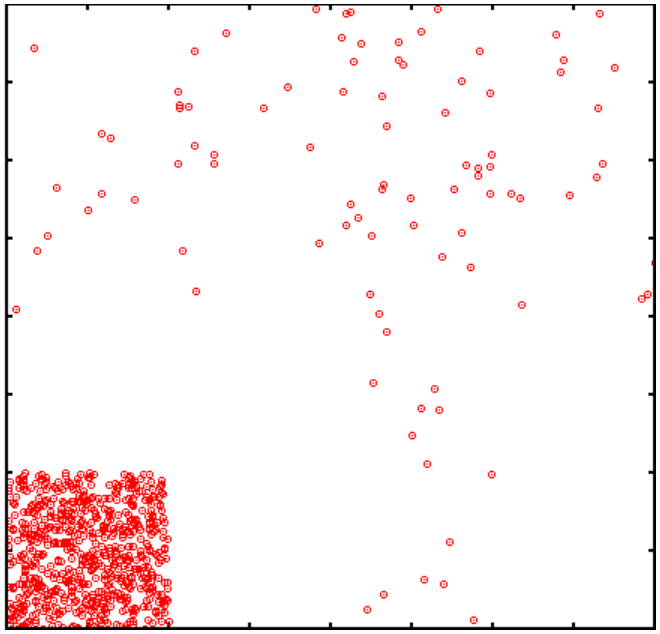
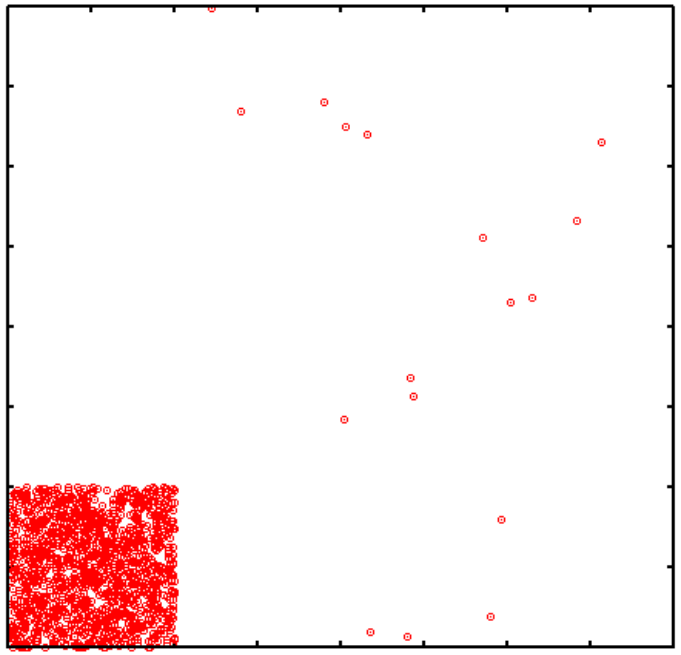
Temperature: 300K





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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