Atomistic modeling of damage production and accumulation in irradiated metals

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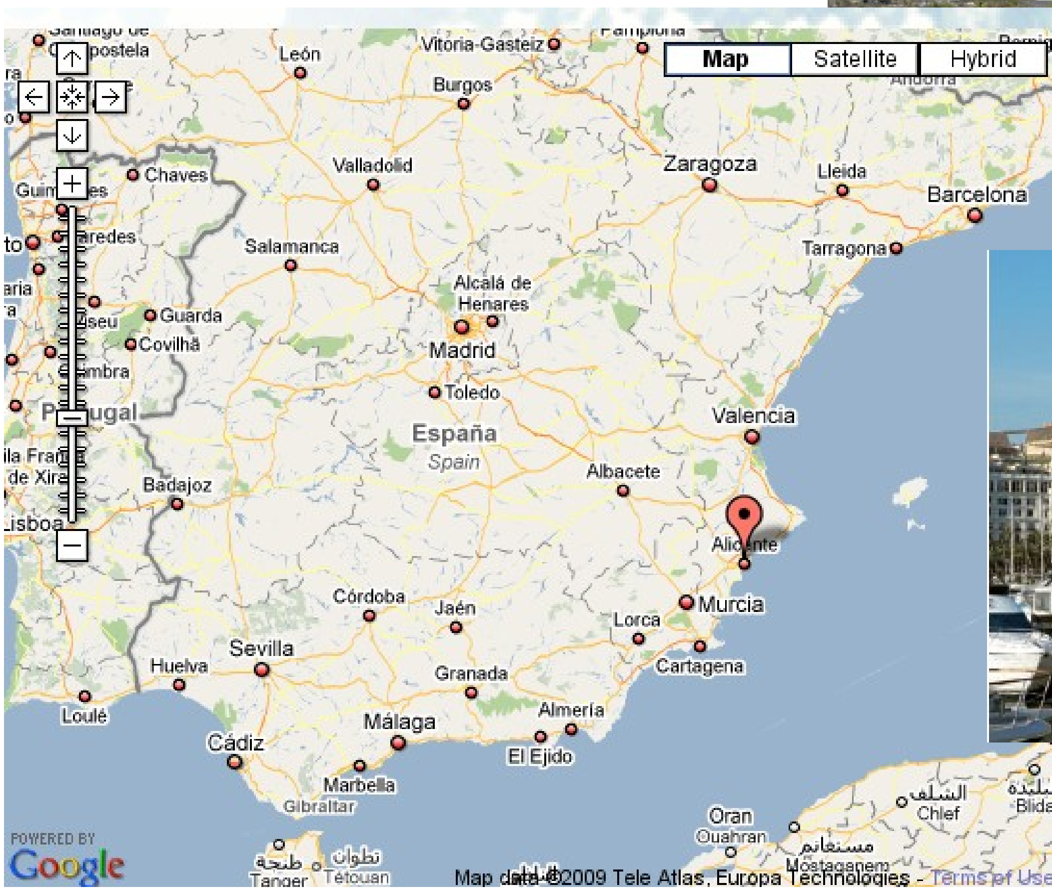

Collaborators and co-authors

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- **K. Nordlund,** University of Helsinki
- **M. J. Aliaga**, UA
- **Anna Prokhodseva, R. Schaeublin, CRPP-EPFL, CH**
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- **L. Malerba**, D. Terentyev, **SCK-CEN, Belgium**
- C. C. Fu & F. Willaime, CEA-Saclay (France)
- B. Gámez, L. Gámez, J. M. Perlado, UPM
- M. Victoria, LLNL (USA)

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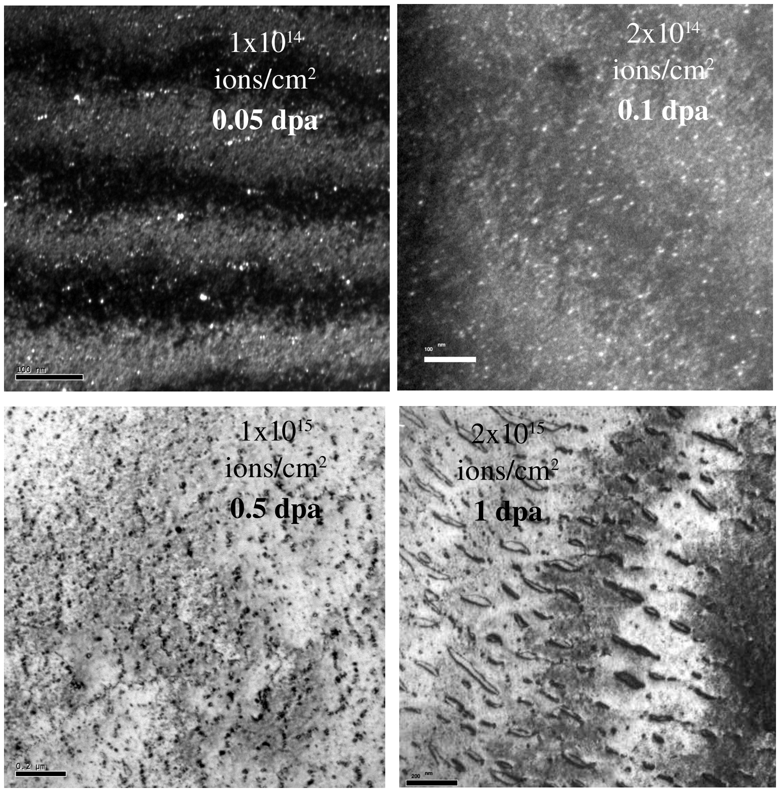
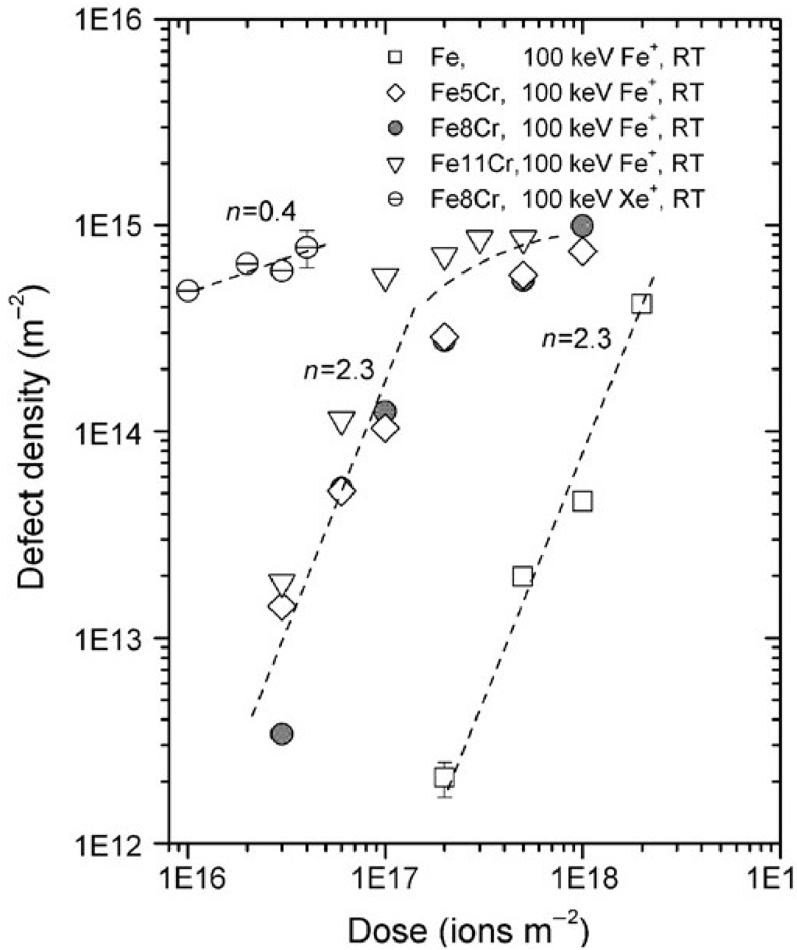
Outline

- Linking ab initio/MD to experiments of irradiation: how to validate the initial conditions?

- Developments in OKMC modeling irradiation of concentrated alloys

Our goal is to reproduce and explain experiments of ion and neutron irradiation in pure metals and alloys



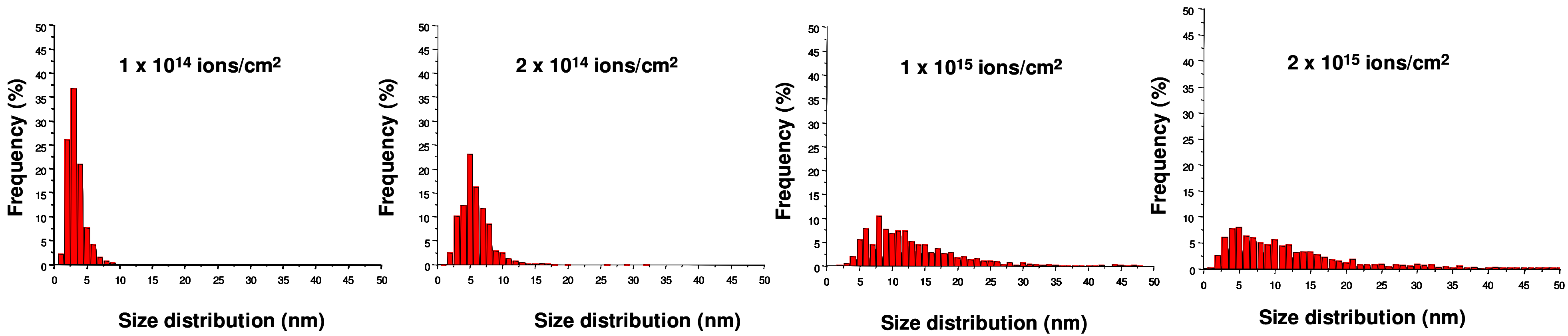


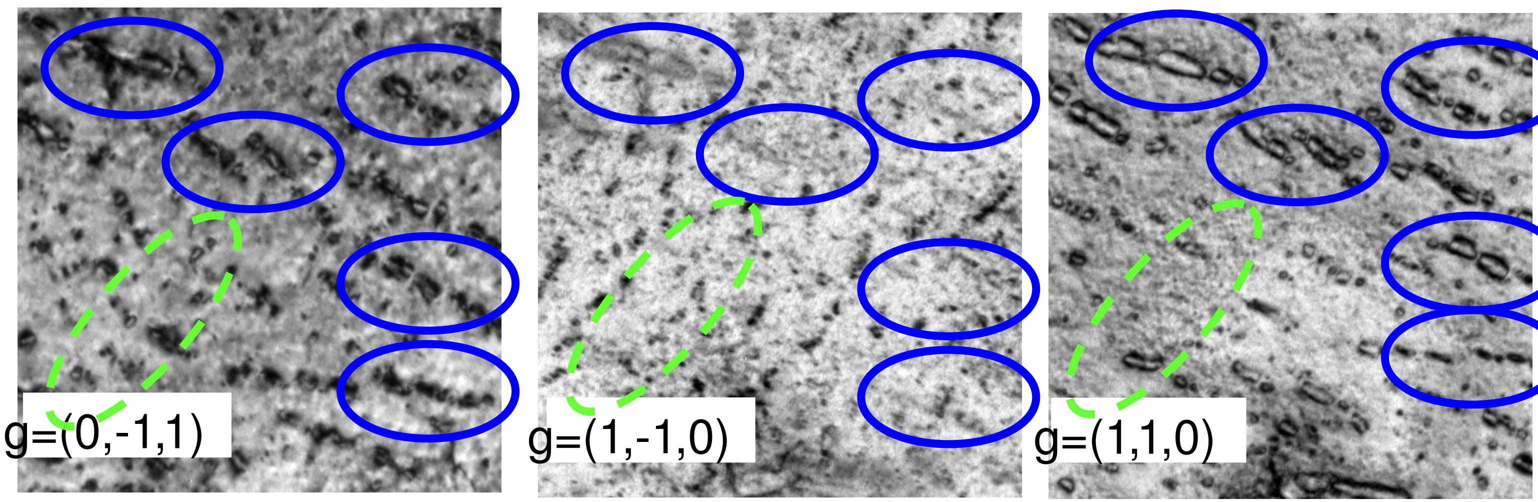
Z. Yao, et al.

Phil. Mag. 88, 2851 (2008)

Ion implantation experiments in Fe and FeCr by
Mercedes Hernández Mayoral (CIEMAT) and co-workers

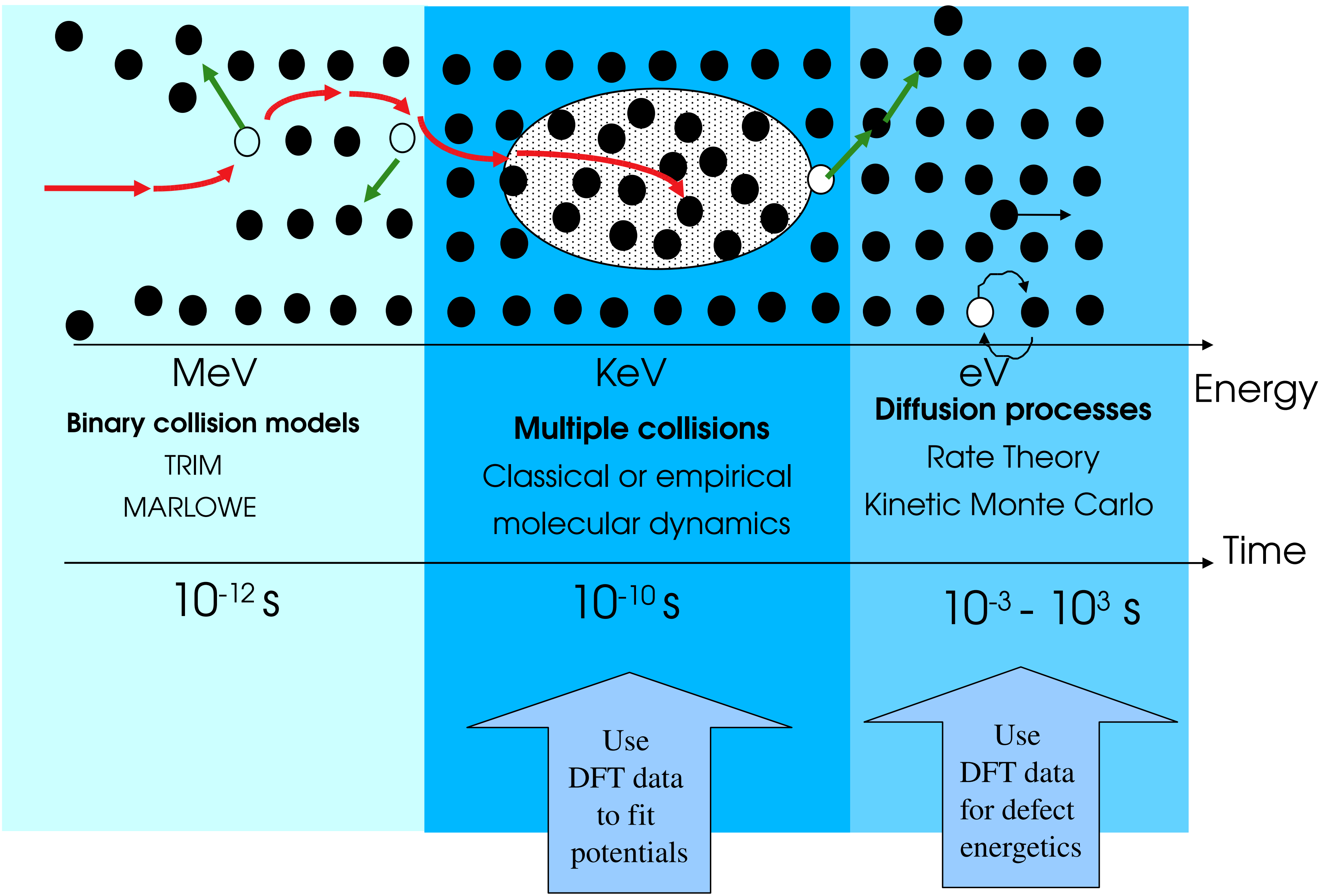
Our goal is to reproduce and explain experiments of ion and neutron irradiation in pure metals and alloys



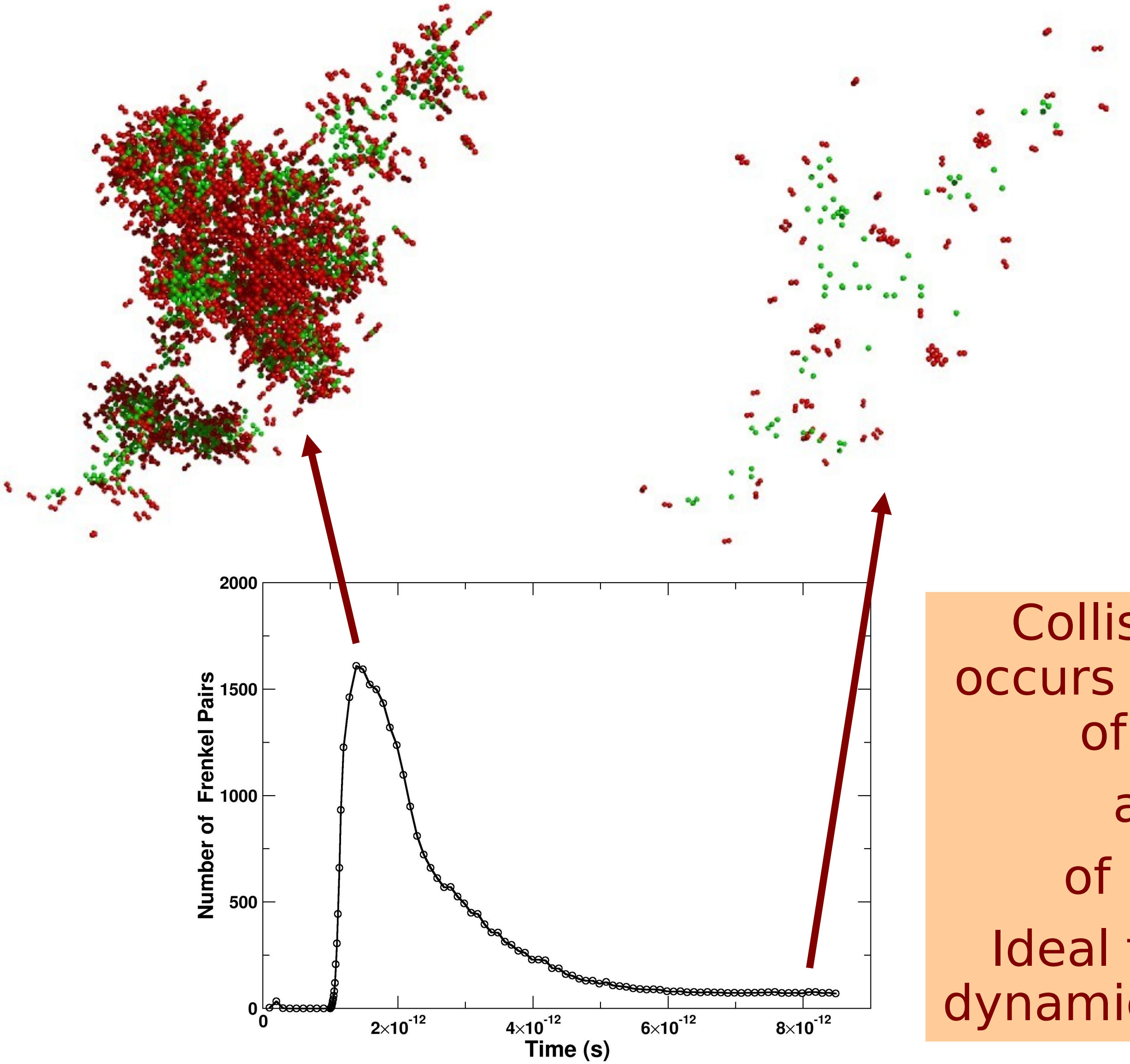


Ion implantation experiments in Fe and FeCr by
Mercedes Hernández Mayoral (CIEMAT) and co-workers

Multiscale modeling is needed to understand radiation damage



First stages of damage produced by a 30keV recoil in Fe



Collision cascade occurs in a time scale of $\sim 10^{-11}$ s

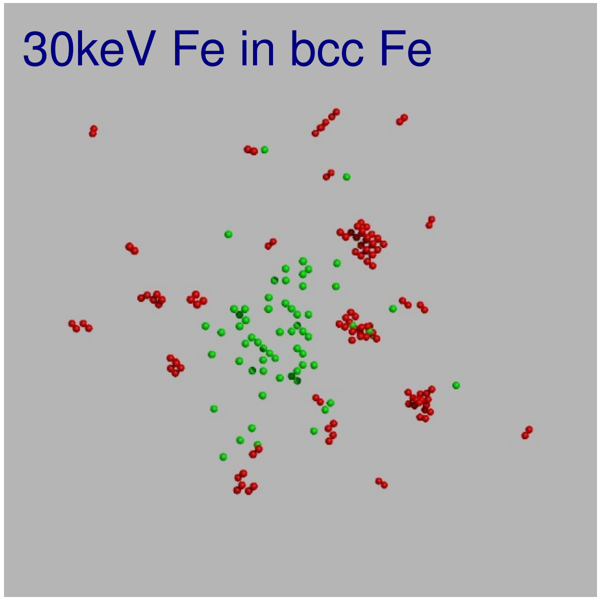
and size

of $\sim (50nm)^3$

Ideal for molecular dynamics calculations

Influence of initial cascade damage distribution (picosecond) on damage accumulation (minutes to hours)

Question addressed: Is the long term evolution of defects affected by the picosecond cascade damage distribution or does it only depend on migration and binding energies of defects?



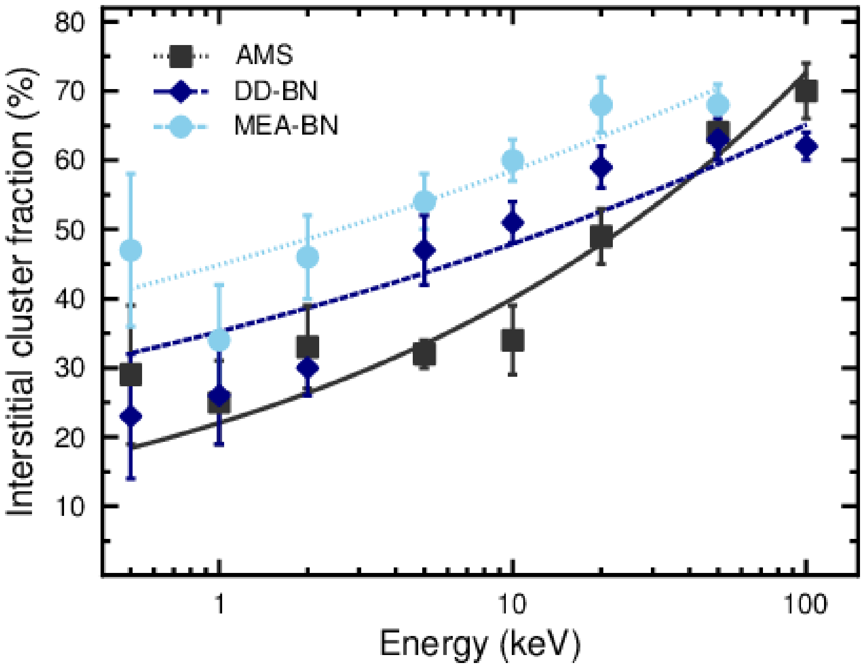
OKMC calculations using cascade damage distributions from 3 different interatomic potentials, AMS [1], DD-BN [2,3] and MEA-BN [3, 4]

[1] G. J. Ackland, M. I. Mendelev, et al. J. Physics: Condens. Matter, 16 (2004) [2] S. L. Dudarev and P. M. Derlet. J. Phys.: Condens. Matter, 17 (2005) [3] C. Bjorkas and K. Nordlund, Nucl. Instrum. & Meth. B 259 (2007) [4] M. Muller, P. Erhart, and K. Albe, J. Phys.: Condens. Matter, 19 (2007)

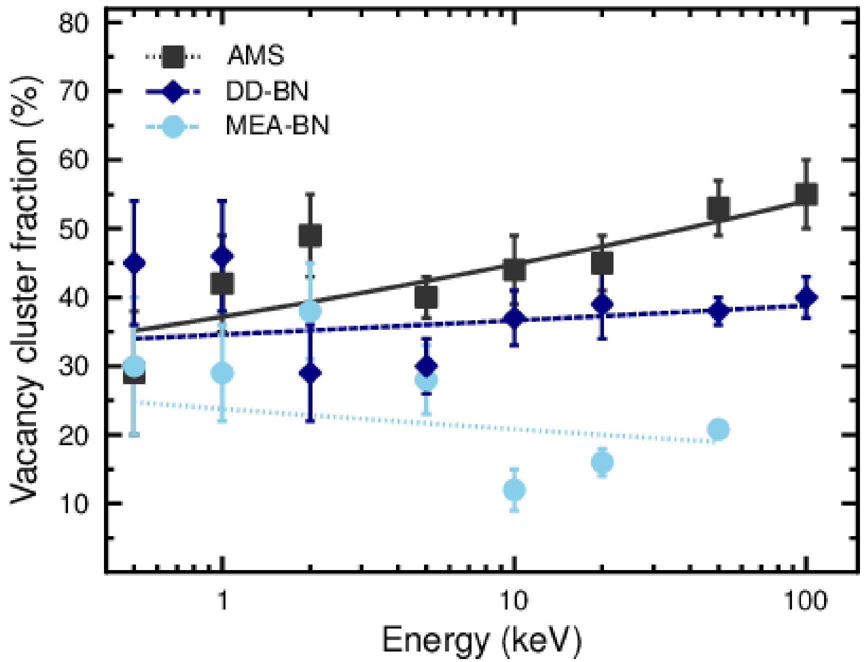
NO EXPERIMENTAL VALIDATION OF MD RESULTS ON SINGLE CASCADE DAMAGE

Differences in defect clustering with int. potential

Interstitials clustered fraction



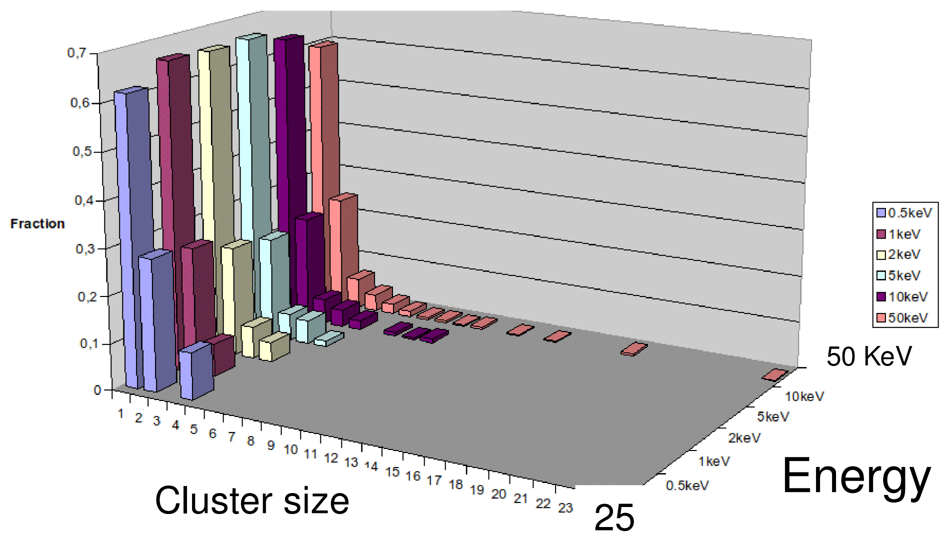
Vacancies clustered fraction



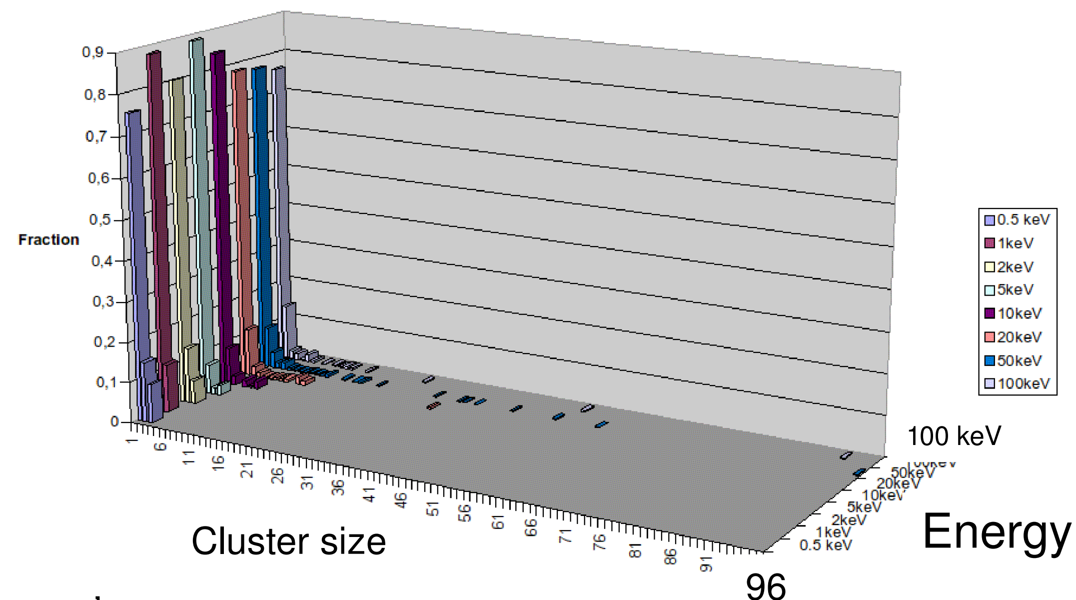
Similar fraction of interstitials in clusters and some differences for vacancies

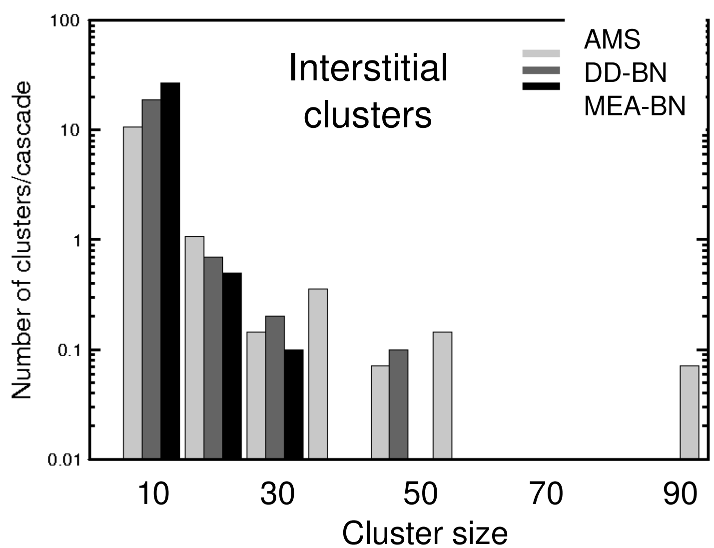
Differences in cluster size distribution with int. potential

SIA MEA Potential



SIA AMS Potential

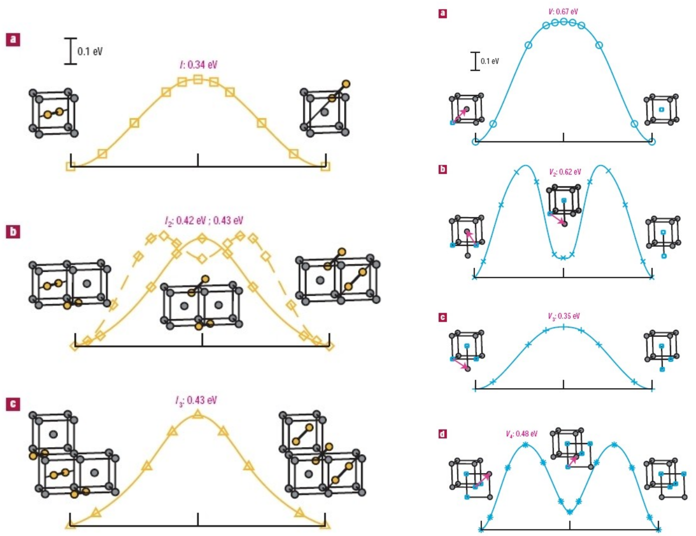




AMS potential predicts significantly larger self-interstitial clusters at 50keV cascades

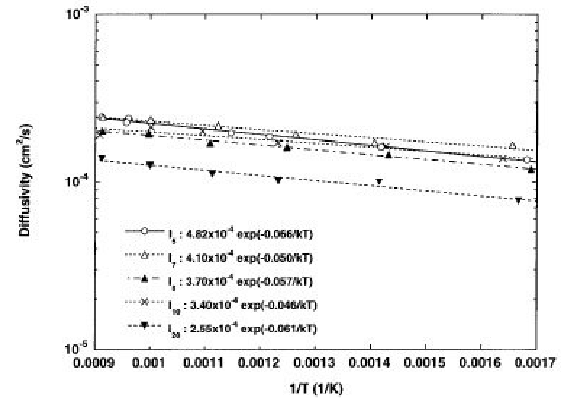
OKMC parameters for Fe

Stabilities and mobilities of vacancies and self-interstitials and their clusters
DFT



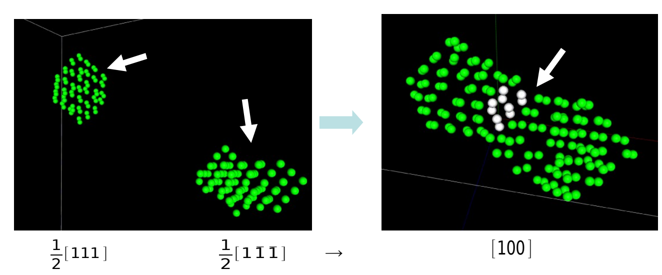
Chu Chun Fu et al. Nature Materials 2005

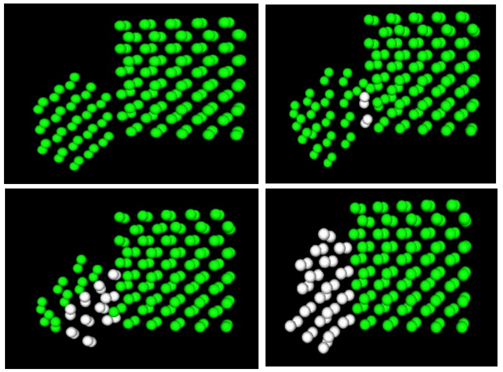
Large clusters or
Interactions between defects:
MD-empirical potentials



Soneda et al. Phil. Mag 2001

1D migration





J. Marian, Phys. Rev. Lett.

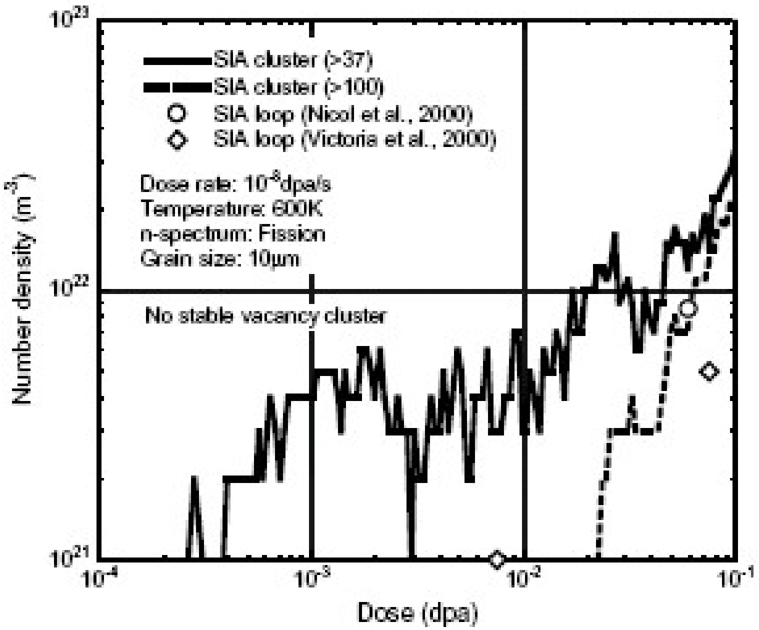
Differences in cluster size distribution with int. potential

Object kinetic Monte Carlo calculations of damage accumulation

Mobilities and binding energies for small vacancy and interstial clusters from DFT [1]

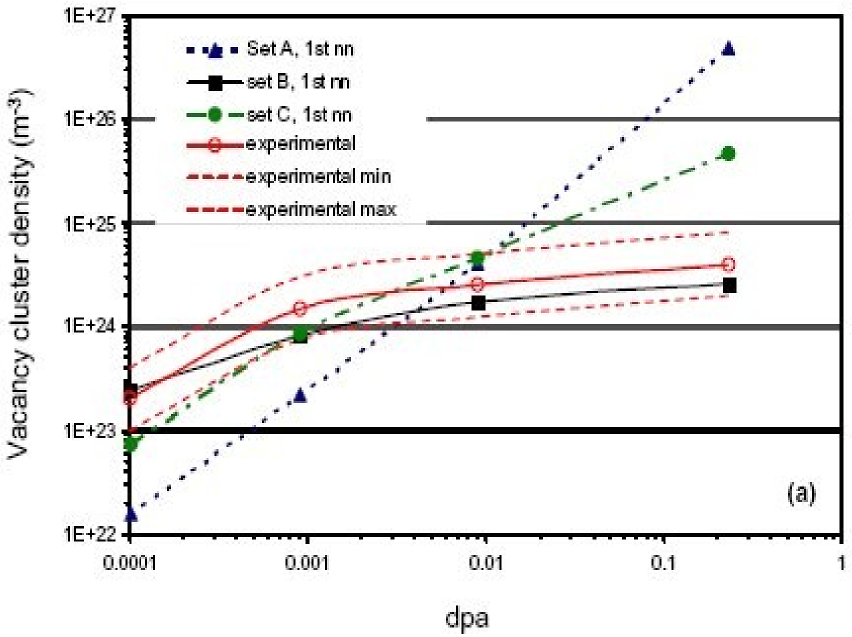
1) All I > 5 immobile
2) Mobilities for I > 5 from MD simulations [2] (<111>) but traps included (0.9 eV)

N. Soneda et al.
J. Nucl. Mat. 2003



Interstitial clusters > 20 immobile

C. Domain et al.
J. Nucl. Mat. 2004



All self-interstitial clusters mobile but traps present

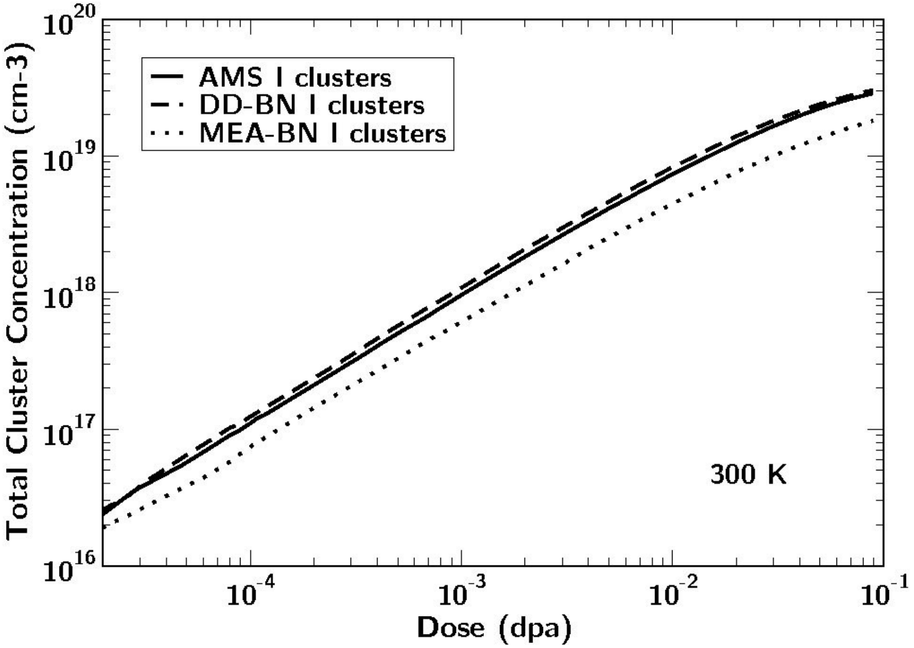
Influence of initial cascade damage distribution on damage accumulation

OKMC simulations

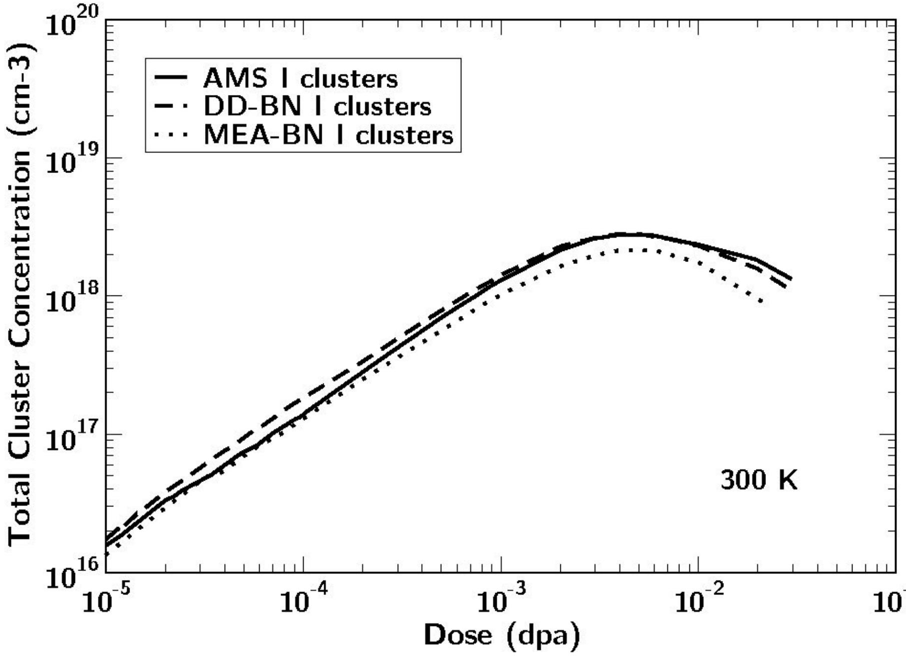
TOTAL DEFECT CONCENTRATION:

no significant difference between the three potentials

I > 5 immobile



I > 5 mobile <111> + traps (0.9 eV)



Influence of initial cascade damage distribution on damage accumulation

VISIBLE DEFECT CONCENTRATION:

only those clusters of interstitials > 55 (loop of 1nm radius)

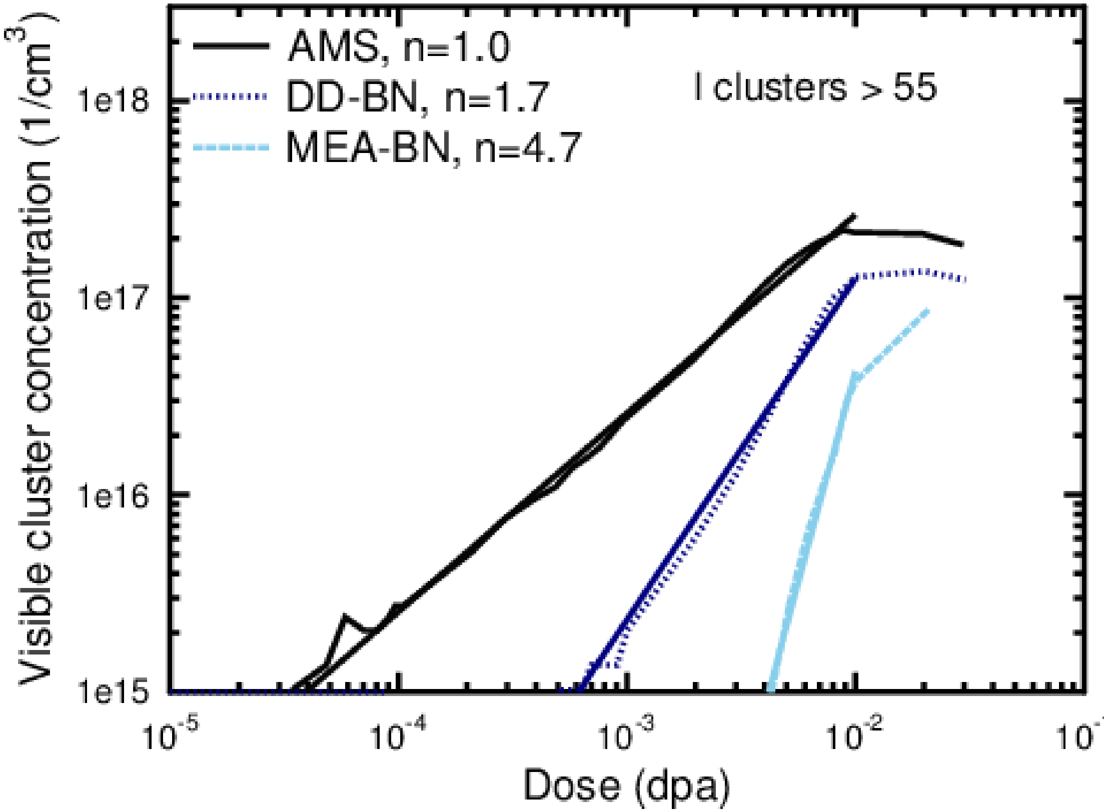
only those clusters of vacancies > 350 (void of 1nm radius)

I > 5 mobile <111>
+ traps (0.9 eV)

Fit to:

$$C = \Phi^n$$

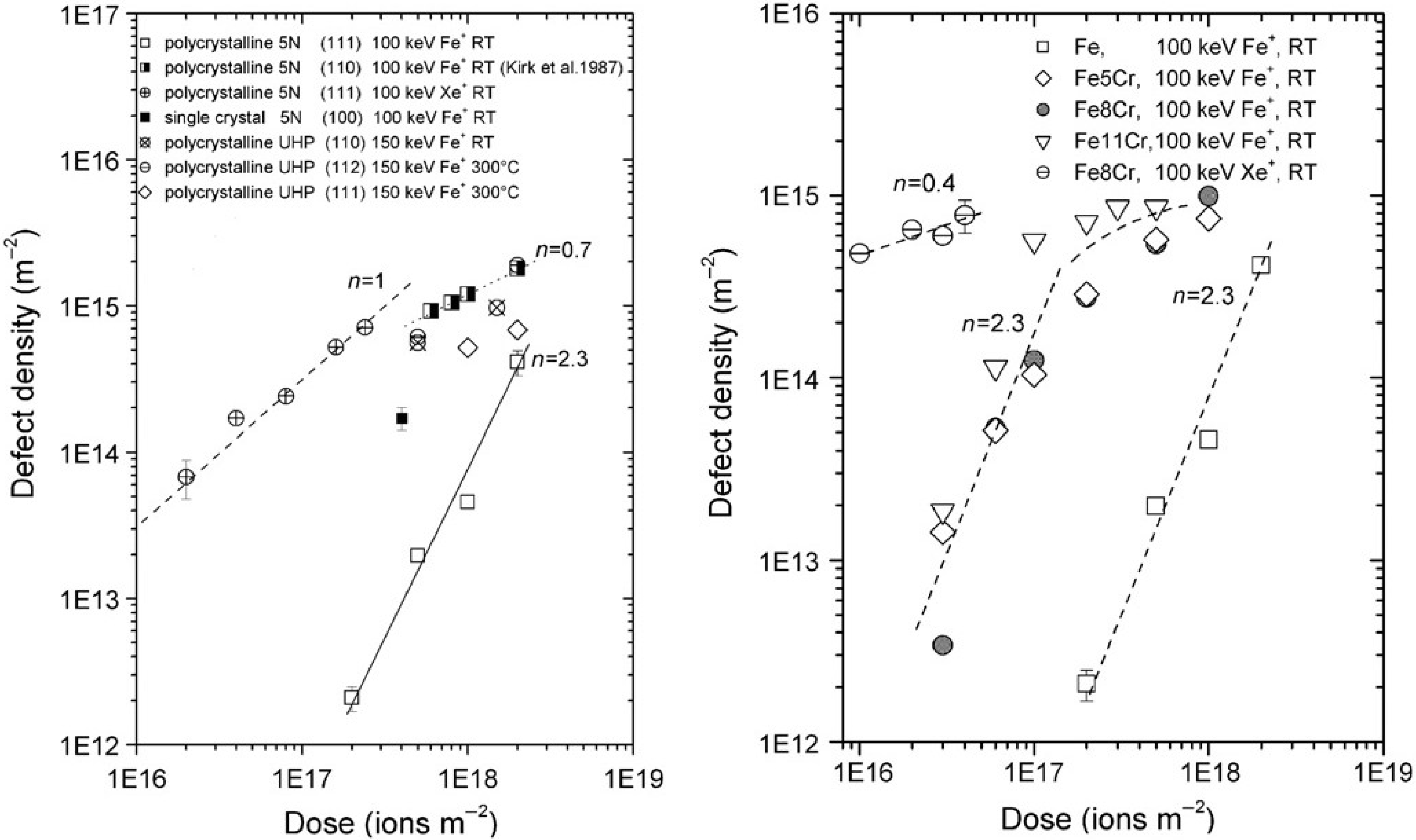
C = concentration
Φ = dose



Björkas, et al. Phys.Rev. B (2012)

Large differences are now observed between the three potentials

Ion implantation experiments in Fe and FeCr by Mercedes Hernández Mayoral (CIEMAT) and co-workers



Can we indirectly validate the MD results of cascade damage distribution?

Ion implantation experiments: thin films?

The JANNuS is a multi-ion beam irradiation platform jointly managed by the "Commissariat à l'Energie Atomique" (CEA), the "Centre National de la Recherche Scientifique" (CNRS) and the "Université Paris-Sud 11" (UPS).

JANNuS has been established on two neighbouring sites:

* At CEA Saclay, a triple ion beam facility
* At CSNSM Orsay allows in-situ observation of the material microstructure modifications induced by ion irradiation/implantation.

http://jannus.in2p3.fr/

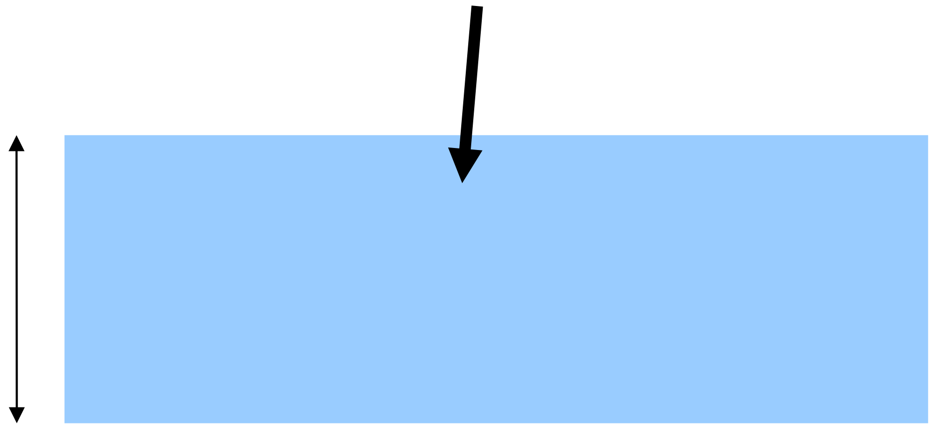
Current experiments by EPFL-CRPP: implantation with ions between 300-500keV in Fe and FeCr alloys and in-situ observations (Anna Prokhodtseva & Robin Schaeublin)

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)

Molecular dynamics simulations of Fe implantation in Fe
Energies: 100 – 500 keV
Inelastic energy loss: Lindhard model
Sample thickness: 40 – 80 nm
Calculations with MDCASK at Juelich HPC-FF supercomputer
Interatomic potentials: DD, AM

40-80nm



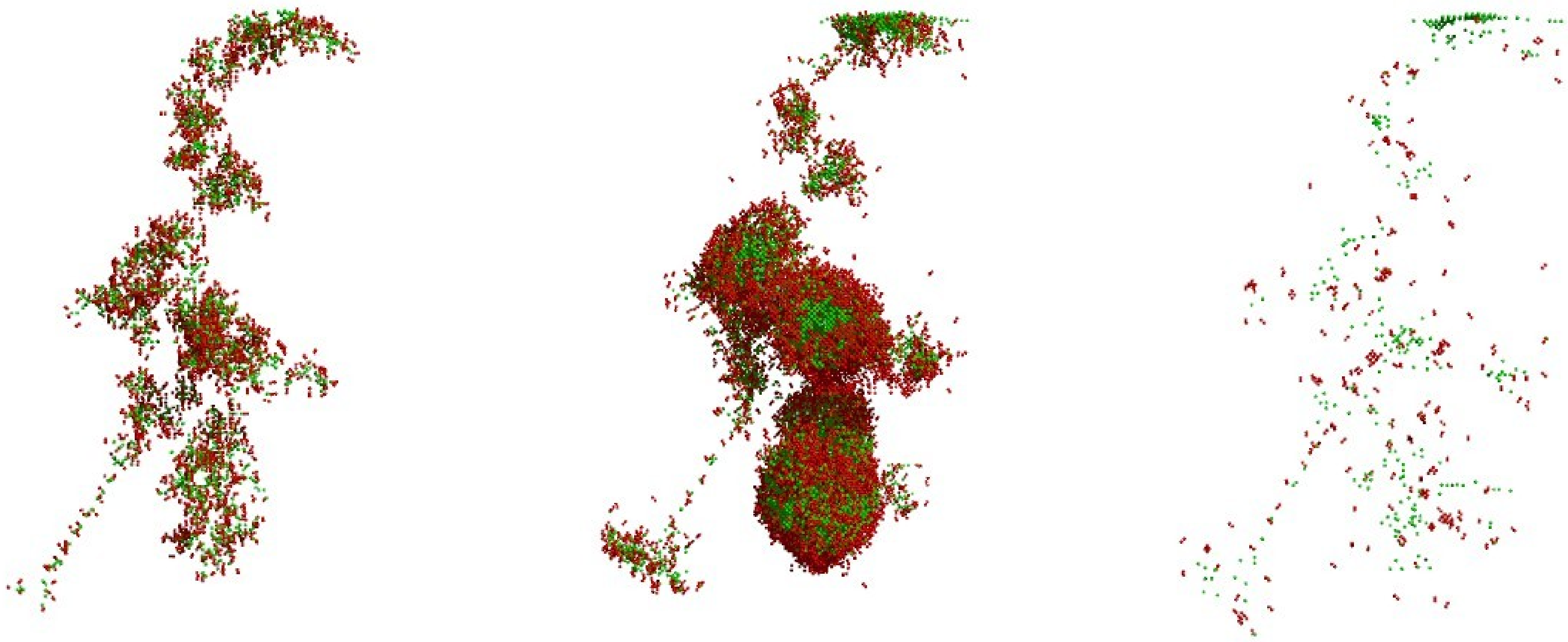
Accurate description of the initial damage to link to in-situ TEM experim.

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)

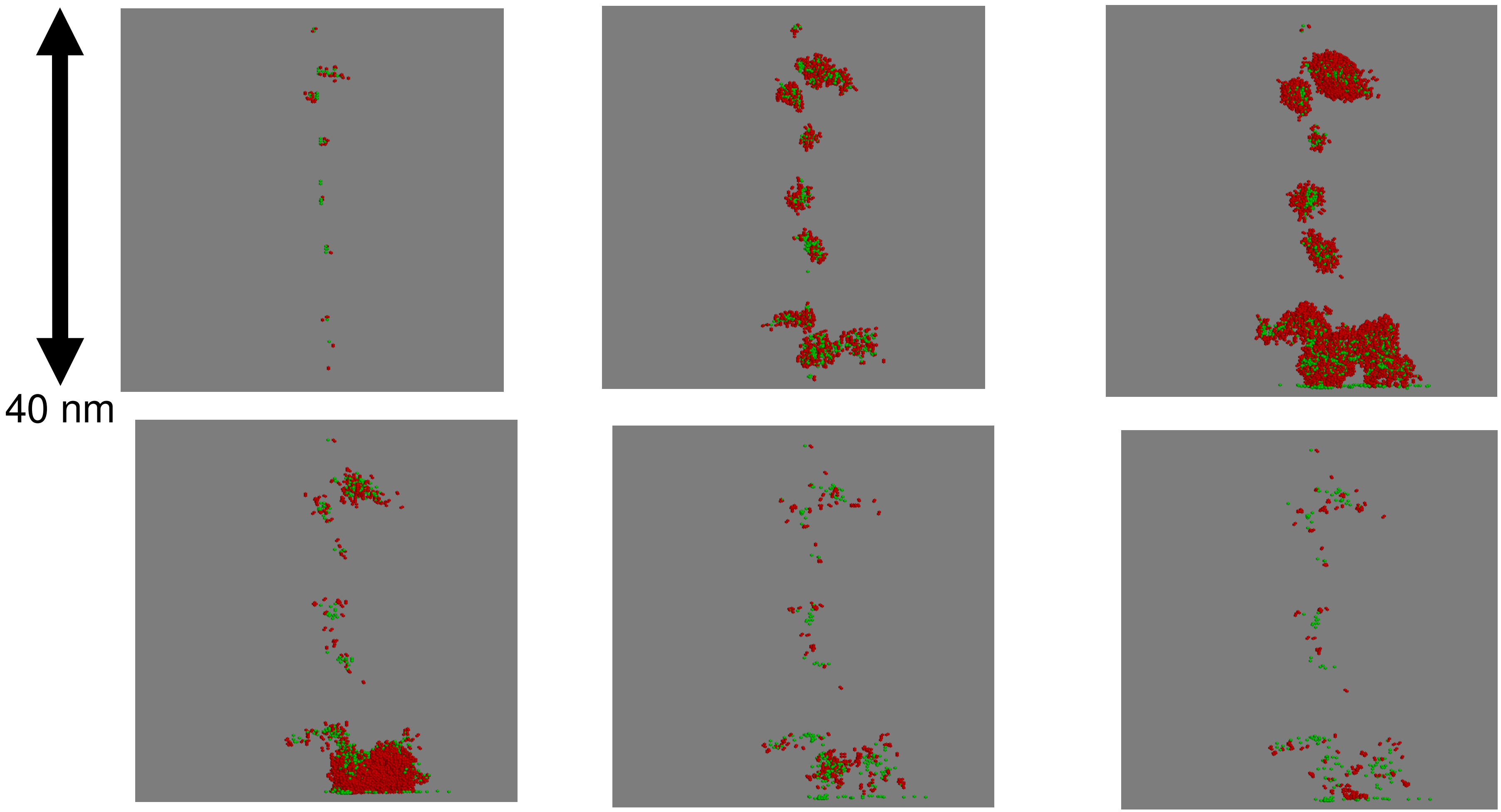
150 keV Fe in Fe

80nm thickness



Accurate description of the initial damage to link to in-situ TEM experim.

Ion implantation in thin films for in situ TEM
Cascade damage for 500keV Fe in Fe, 40nm
Anna Prokhodseva & R. Schaeublin (CRPP-EPFL), M. J. Aliaga(UA)

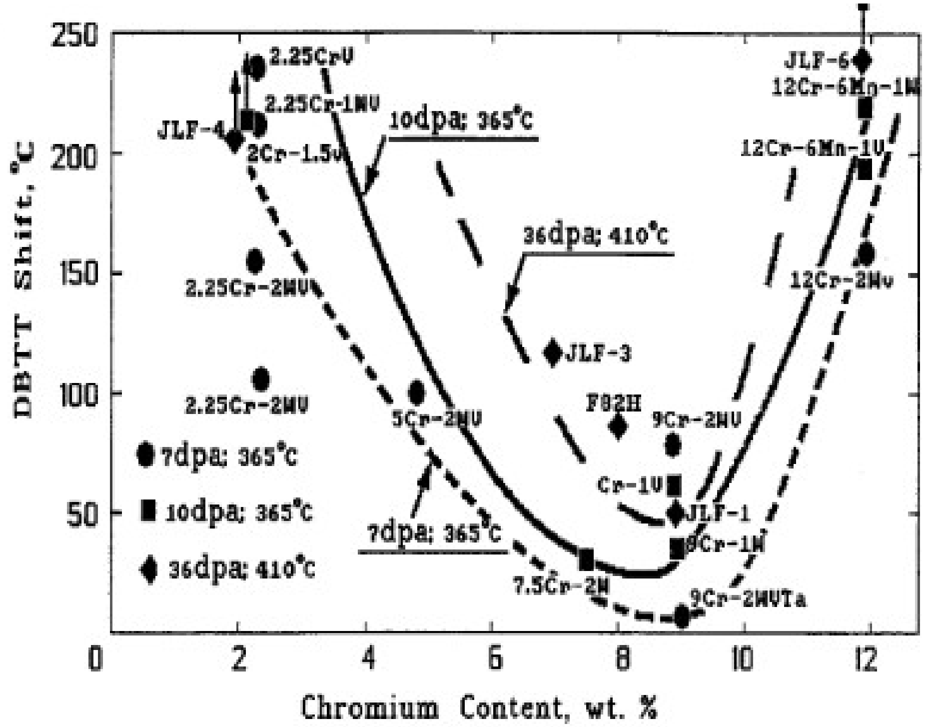


Accurate description of the initial damage to link to in-situ TEM experim.

Key issues of radiation effects in Fe-Cr alloys

- How do mechanical properties change with Cr content?
- Non monotonic behaviour observed in some cases

DBTT Shift as a function of Cr content



Kohyama et al. JNM, 233-237 (1988) 138

Increased loop density in FeCr vs. Fe

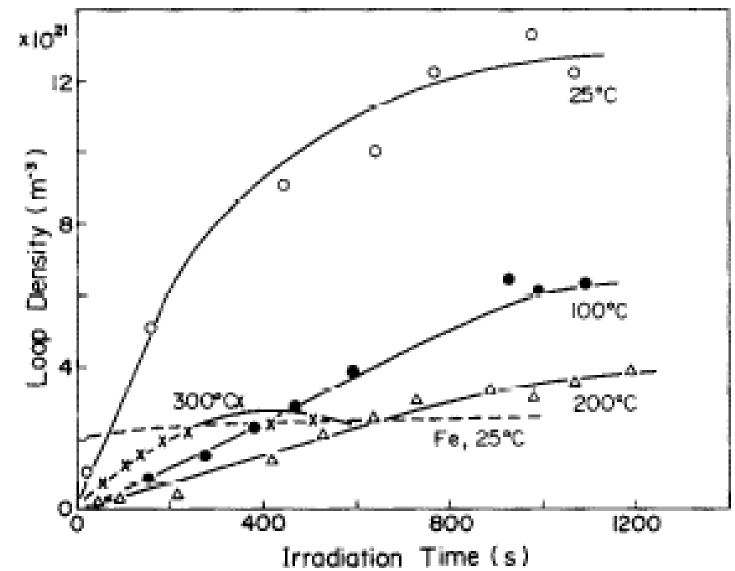


Fig. 2. Irradiation time dependence of loop density in Fe–10% Cr alloy at several temperatures. The data for Fe at 25° C are also shown for comparison.

Yoshida, 1988, JNM

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

Long term evolution of FeCr alloys

Challenge: reach the time and length scales needed

- What can be done with the OKMC codes today?
  - Generally sizes of $(0.2\mu m)^3$ with PBC, or up to $2\mu m$ in one direction
  - Dose up to 0.5 to 1 dpa (CPU times of days to weeks)

- Where do we need to go?
  - Keep at least the same simulation sizes
  - High doses – beyond 1 dpa
  - High temperatures (up to 600°C)

- What are the specific challenges of FeCr?
  - Concentration of Cr: in a $(0.2\mu m)^3$ box, Fe9Cr ~ 60 Million Cr !!
  - Precipitates: sizes of 100s of nms

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:

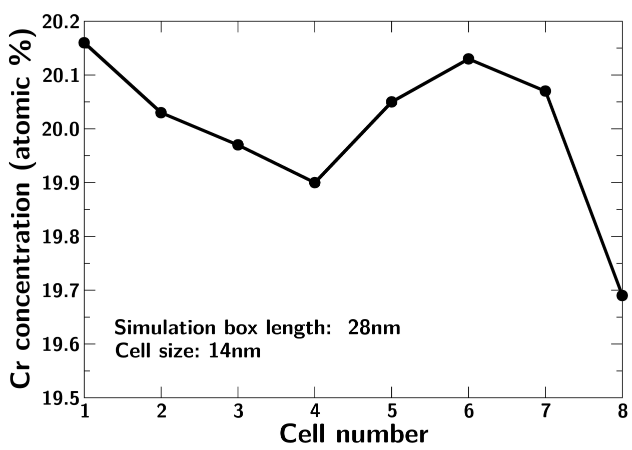
Cr represented in terms of average local concentration
OKMC simulation box divided into smaller boxes (cells) with different Cr concentration
Initial Cr distribution random in the simulation box
Two new input parameters in the simulation: Concentration of the alloy (in atomic %) and number of cells in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

C_1	C_2	…
…	C_i	C_{i+1}
	…	C_N

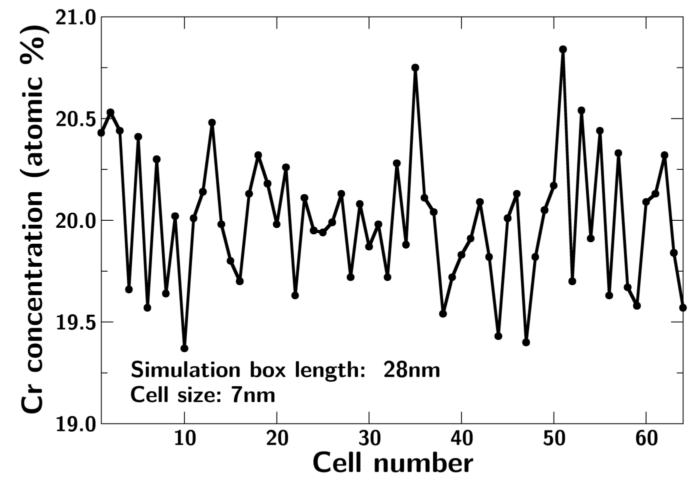
Example: Concentration of Cr in each cell

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 <u>and concentration of neighboring cells:</u>

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

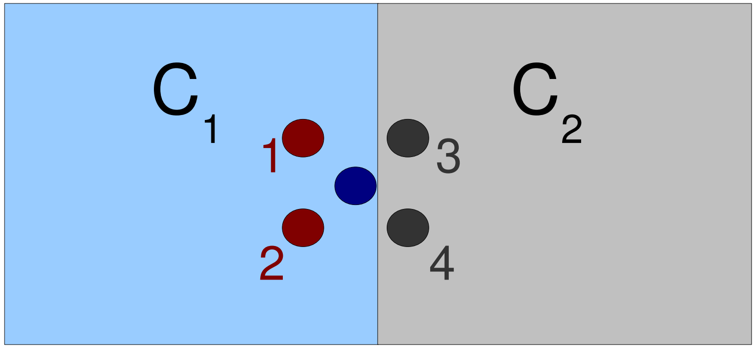
The same process has to be done every time a vacancy jumps to a new location

Implementation steps

Step 3:

Example:

A vacancy is created in cell 1 with alloy concentration C_1



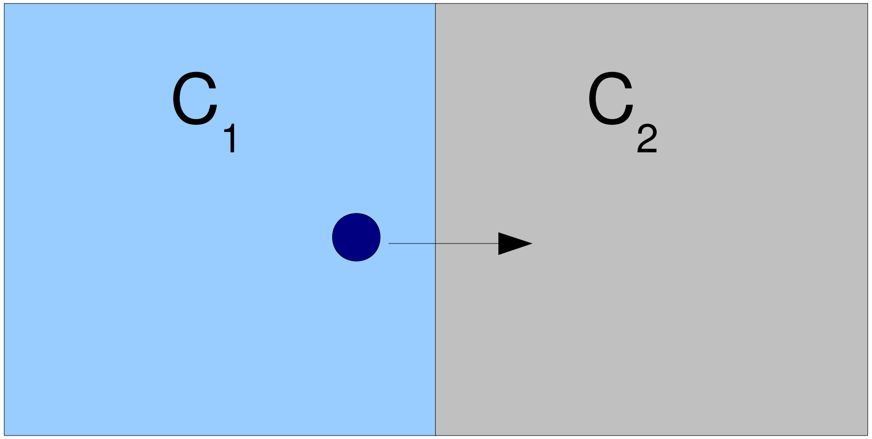
- The location of all neighbors is determined (BCC lattice) and the type of neighbor
- The probability of that vacancy jumping to any of its nearest neighbors is evaluated depending on the location and type of the neighbors.

For example: the migration energy could be: E_m^0 + w(c2-c1) such that the jump is favored if C1 > C2. (An alloy atom will move from C2 to C1 increasing the concentration in 1 and decreasing the concentration in 2).

Implementation steps

Step 4:

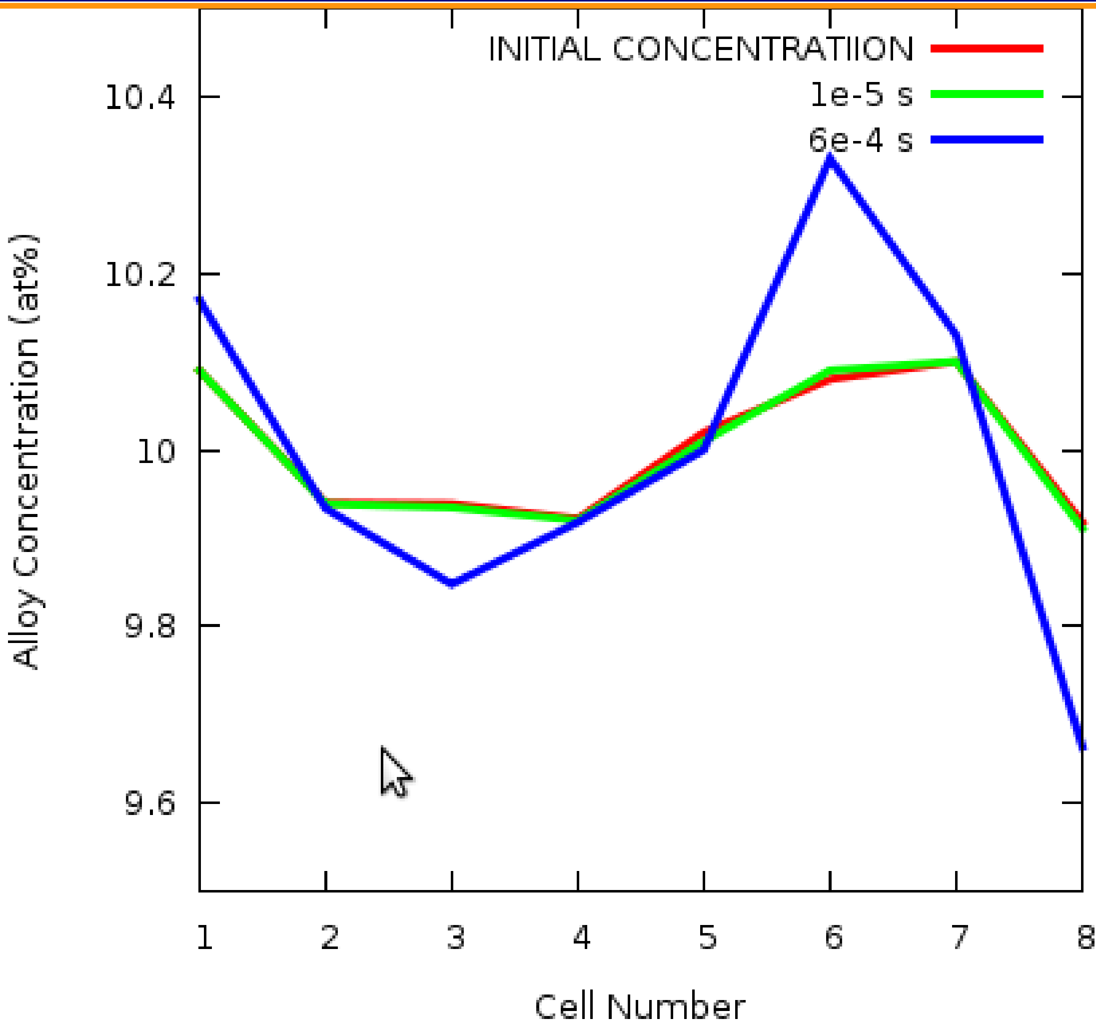
After a vacancy jumps the concentration of the alloy or the matrix element in the original cell where the vacancy was located and the final cell where the vacancy jumped has to be evaluated



Test runs

Test 1:

Alloy concentration: 10 atomic%
Vacancy concentration:
1 vacancy in the whole box
Simulation box:
28.6nmx28.6nmx28.6nm
Number of cells: 8 (2x2x2)
Temperature: 600K

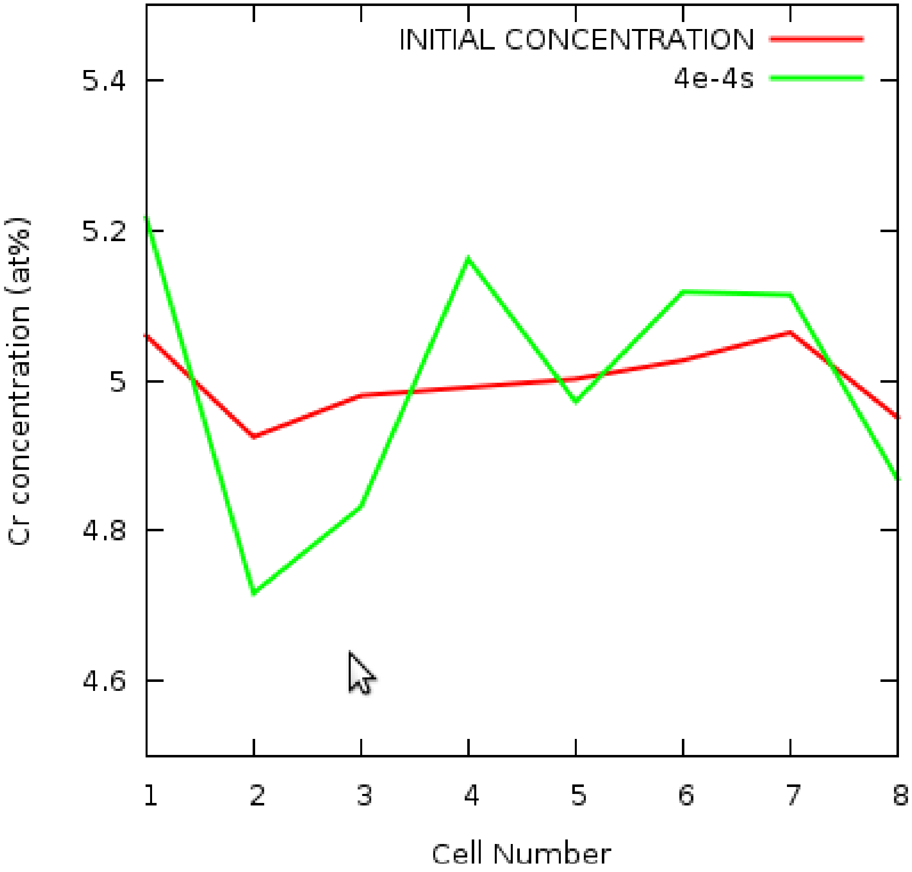


We start with an inhomogeneous distribution of Cr
Cr moves from the lowest concentration cells to the highest concentrations

Test runs

Test 1:

Alloy concentration: 5 atomic%
Vacancy concentration:
1 vacancy in the whole box
Simulation box:
28.6nmx28.6nmx28.6nm
Number of cells: 8 (2x2x2)
Temperature: 600K



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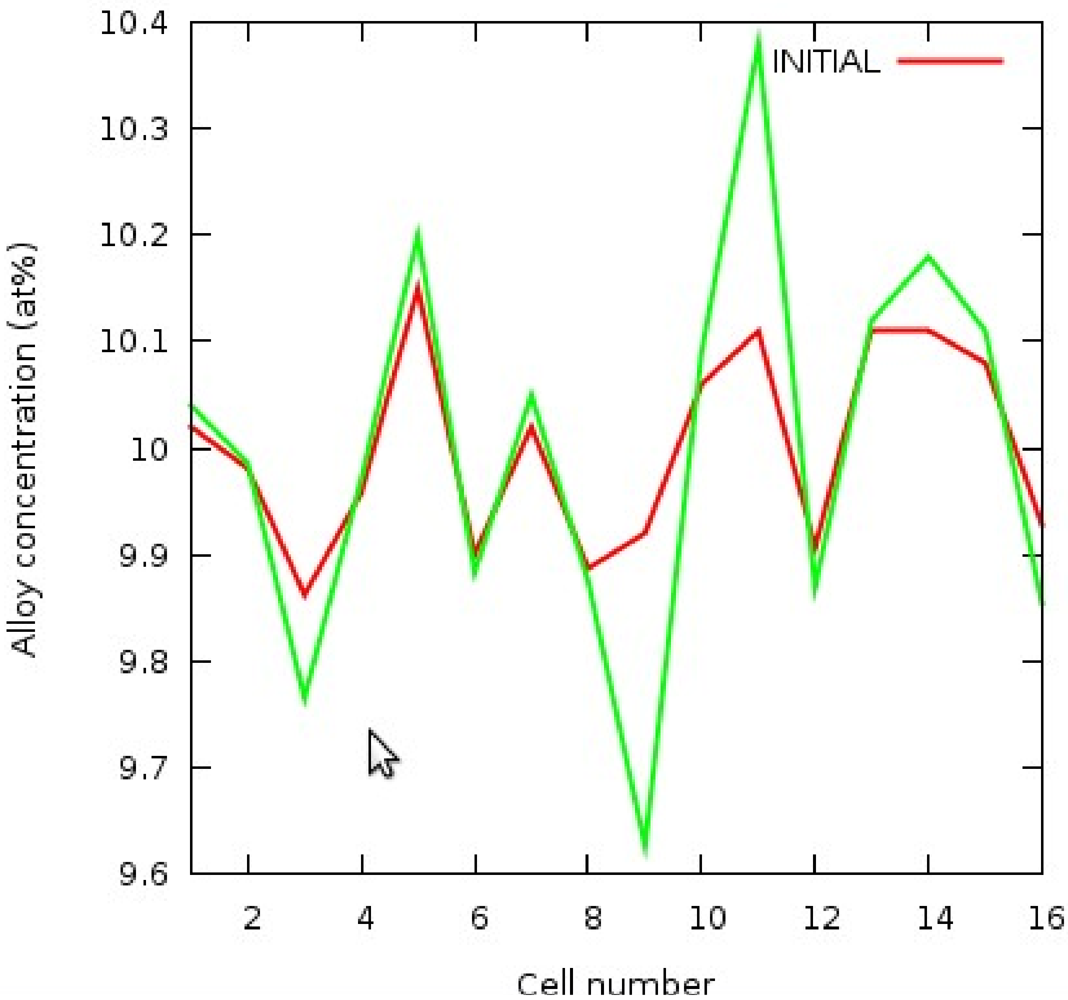
Test runs

Test 1:

Alloy concentration: 10 atomic%
Vacancy concentration:
1 vacancy in the whole box
Simulation box:
28.6nmx28.6nmx28.6nm
Number of cells: 16 (4x2x2)
Temperature: 600K



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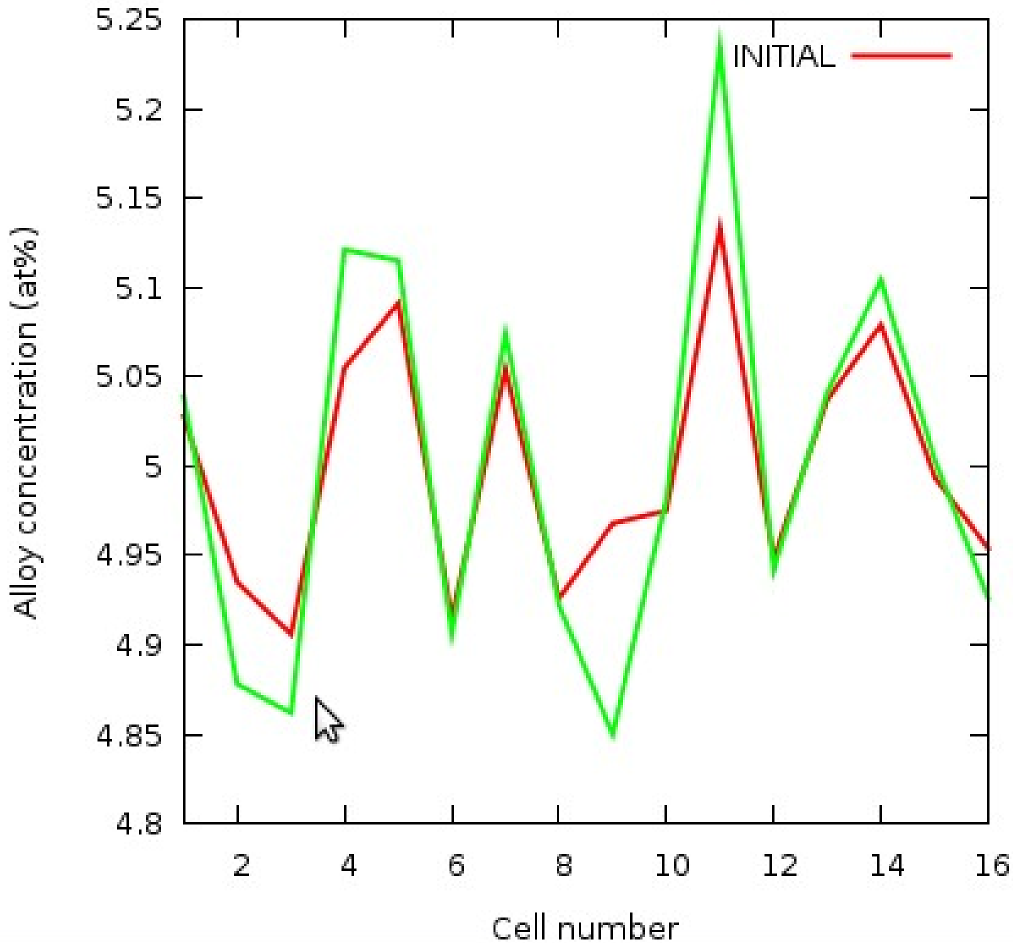


We start with an inhomogeneous distribution of Cr
Cr moves from the lowest concentration cells to the highest concentrations

Conclusions and on-going work

- •Picosecond damage distribution is propagated over long time scales: importance of the “correct” initial damage distribution (“butterfly effect”)
- •Can we validate the ps damage distribution from MD with long timescale MD+OKMC vs. experiments?
- •A first implementation of a combination of continuous alloy concentration and discrete defect diffusion is on the way
- •Taking into account the diffusion of alloy atoms and biasing the migration according to local concentrations we can observe precipitation

OKMC: methodology

Input Data

Defect Distribution → From MD

Rate for each Event R_i →
- Defect Jump: *Migration Energy*
- Cluster Dissolution: *Binding Energy*
- New Cascade: *Dose Rate*

Total Rate, R: $\sum R_i \, x \, N_i$ with Ni number of particles for Event i

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

Update Time: Time = -log (random)/R

Do Event: find neighbours of atoms that moved

Until final time or dose

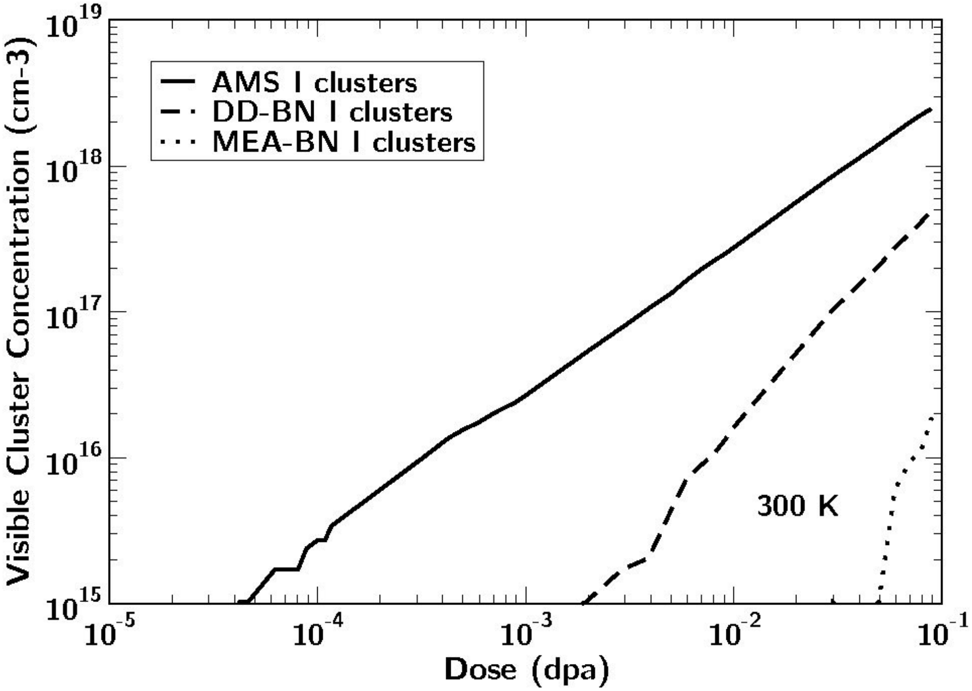
Influence of initial cascade damage distribution on damage accumulation (Carolina Björkas, Univ. Helsinki)

VISIBLE DEFECT CONCENTRATION:

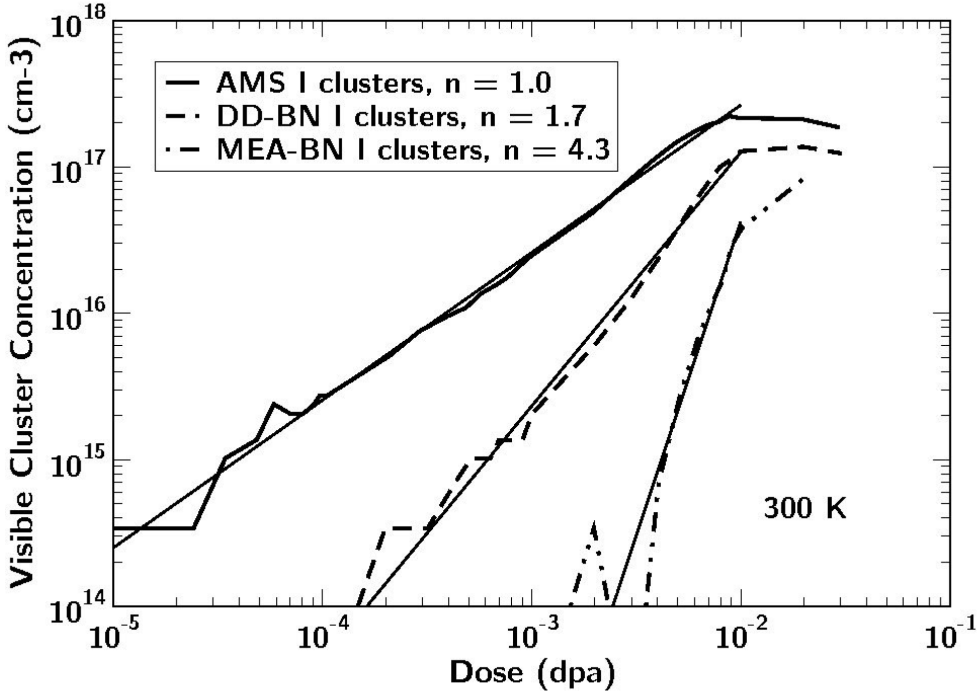
only those clusters of interstitials > 55 (loop of 1nm radius)

only those clusters of vacancies > 350 (void of 1nm radius)

I > 5 immobile



I > 5 mobile <111> + traps (0.9 eV)



Large differences are now observed between the three potentials