Fusion HPC Workshop

Vacancy and self-interstitial assisted migration of Cr in FeCr alloys

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Radiation Induced Segregation

The main goal is to obtain a model that can reproduce radiation induced segregation as observed in experiments with FeCr alloys:

- enrichment/depletion of Cr near grain boundaries
- decoration of dislocations with Cr atoms

OKMC model combining the evolution of point defects (PD) produced in irradiated materials, and solute transport due to PD migration according to the thermodynamics of the system.

$$E_m(Cell_1 \rightarrow Cell_2) = E_{m,0} + \frac{\Delta G}{2} \qquad \Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}$$

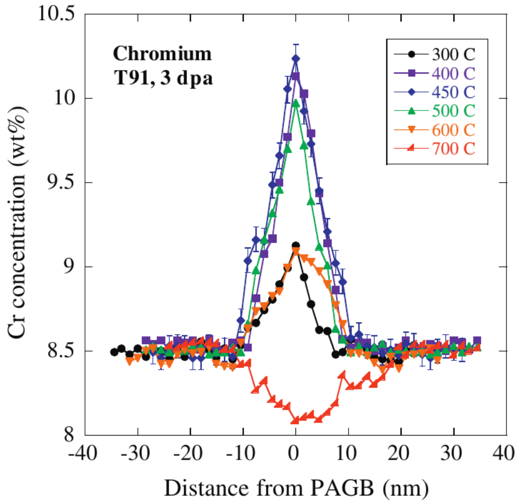
where the total change of free energy is calculated using analytical expressions that depends on $\mathbf{x}_{Cr}$

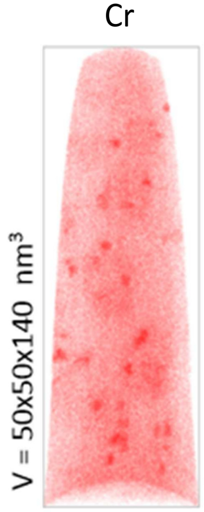
$$\Delta S_{mix} = -k_B[(1-x)\ln(1-x) + x\ln(x)]$$

$$\Delta H_{mix} = -(x-\alpha)(\beta x^2 + \gamma x + \delta)\left(1 - \frac{T}{\Theta}\right)x(1-x)$$

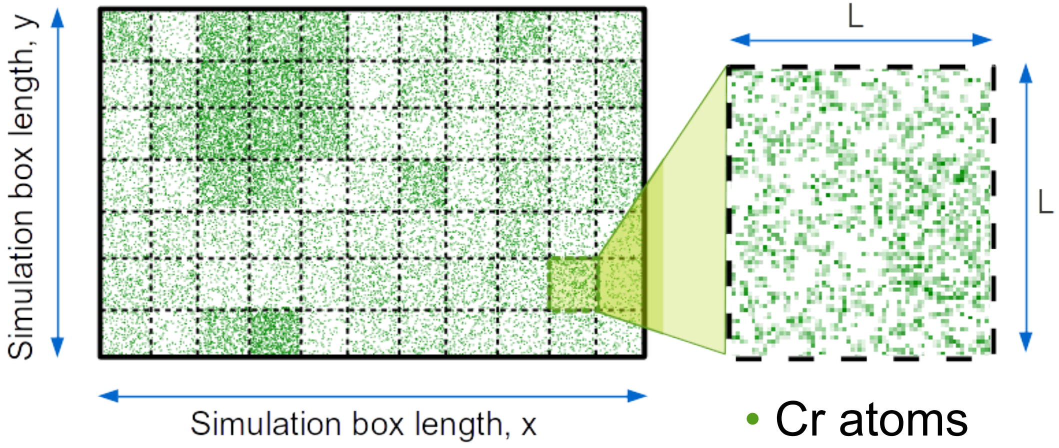
M. Levesque et al. PRB 84 (2011)

J.P. Wharry et al. JNM 442 (2013)





B. Gomez-Ferrer et al. JNM 537 (2020)



J.P. Balbuena et al. JNM 557 (2021)

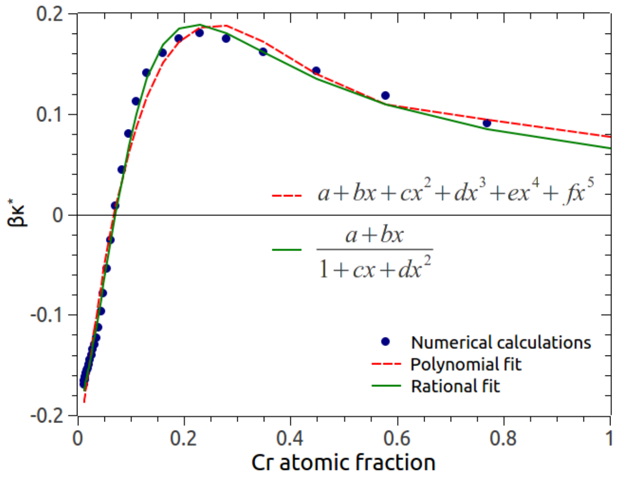
Vacancy assisted migration of Cr

Interface energy term

$$E_{mig}(x) = E^{0}_{mig}(x) + \frac{1}{2}(\Delta E_{homo} + \Delta E_{inhomo})$$

Interaction between 1NN cells controlled by stiffness coefficient $\tilde{\kappa}$

$$E_{inhomo}(x_i) = \frac{1}{2} n_i \tilde{\kappa}(x_i) \sum_{j}^{1NN} (x_i - x_j)^2$$



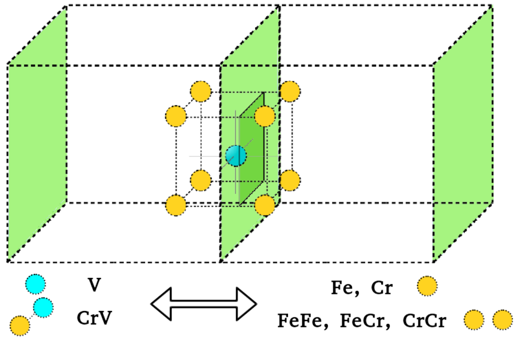
Creation of VCr pairs

Following the execution of a migration event where **V** replaces a **Cr** lattice atom, a **VCr** pair is created with both particles.

$$V + Cr \rightarrow VCr$$

Migration of VCr pairs

VCr migration uses the same algorithn than the one of point defects but featuring additional restrictions considering the populations of Fer and Cr scpecies in both cells.



Exchanges:

$$V \longleftrightarrow Fe$$
$$V \longleftrightarrow Cr$$
$$VCr \longleftrightarrow CrFe$$
$$VCr \longleftrightarrow CrCr$$
$$VCr \longleftrightarrow FeFe$$

Breakup of VCr

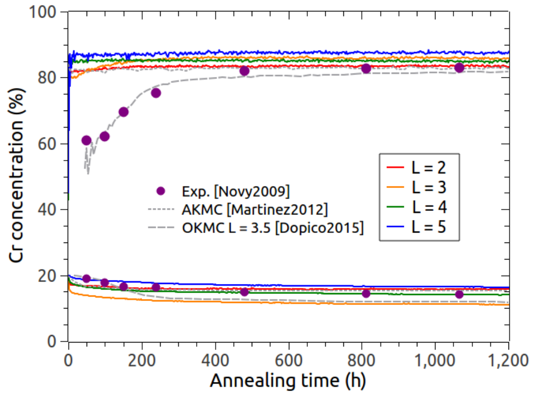
Independent event in the OKMC algorithm using both the VCr binding energy and lifetime.

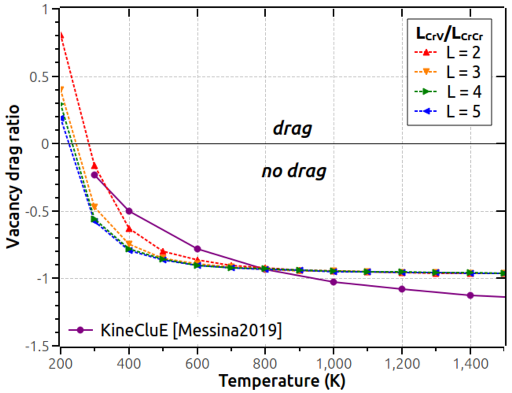
Vacancy assisted migration of Cr

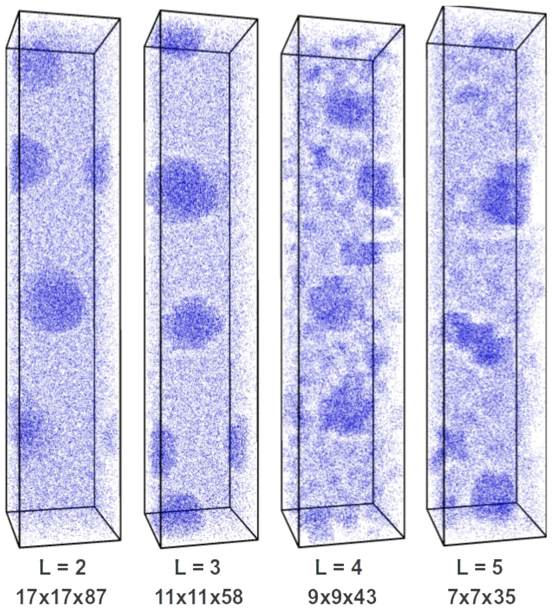
Different cell sizes

Different temperatures

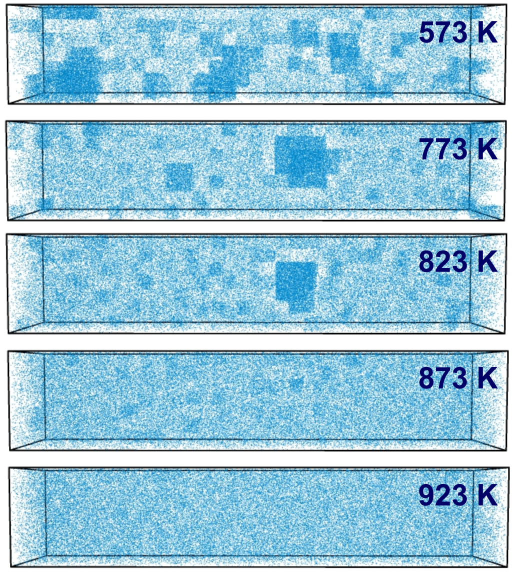
Evaluation of the code with simulations at different temperatures and different cell sizes will verify that the model follows the phase diagram of the FeCr alloy, so that the code not only reports valid outputs for the given temperature 773 K.





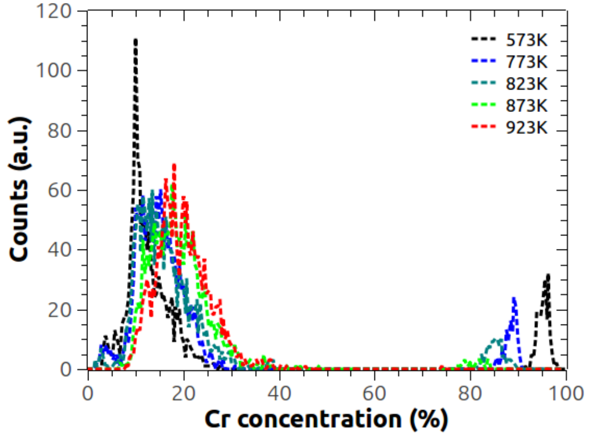


S. Novy et al. JNM 384 (2009)
E. Martinez et al. PRB 86 (2012)



I. Dopico et al. Acta Mat. 95 (2015)
L. Messina et al. Acta Mat. 191 (2020)

Distribution of α and α' phases



Visible Cr precipitates?

	L = 2	L = 3	L = 4	L = 5
573 K	✓	✓	✓	✓
773 K	✓	✓	✓	✓
823 K	✓	✓	✓	✓
853 K	✗	✗	✗	✗
923 K	✗	✗	✗	✗

Self-interstitial assisted migration of Cr

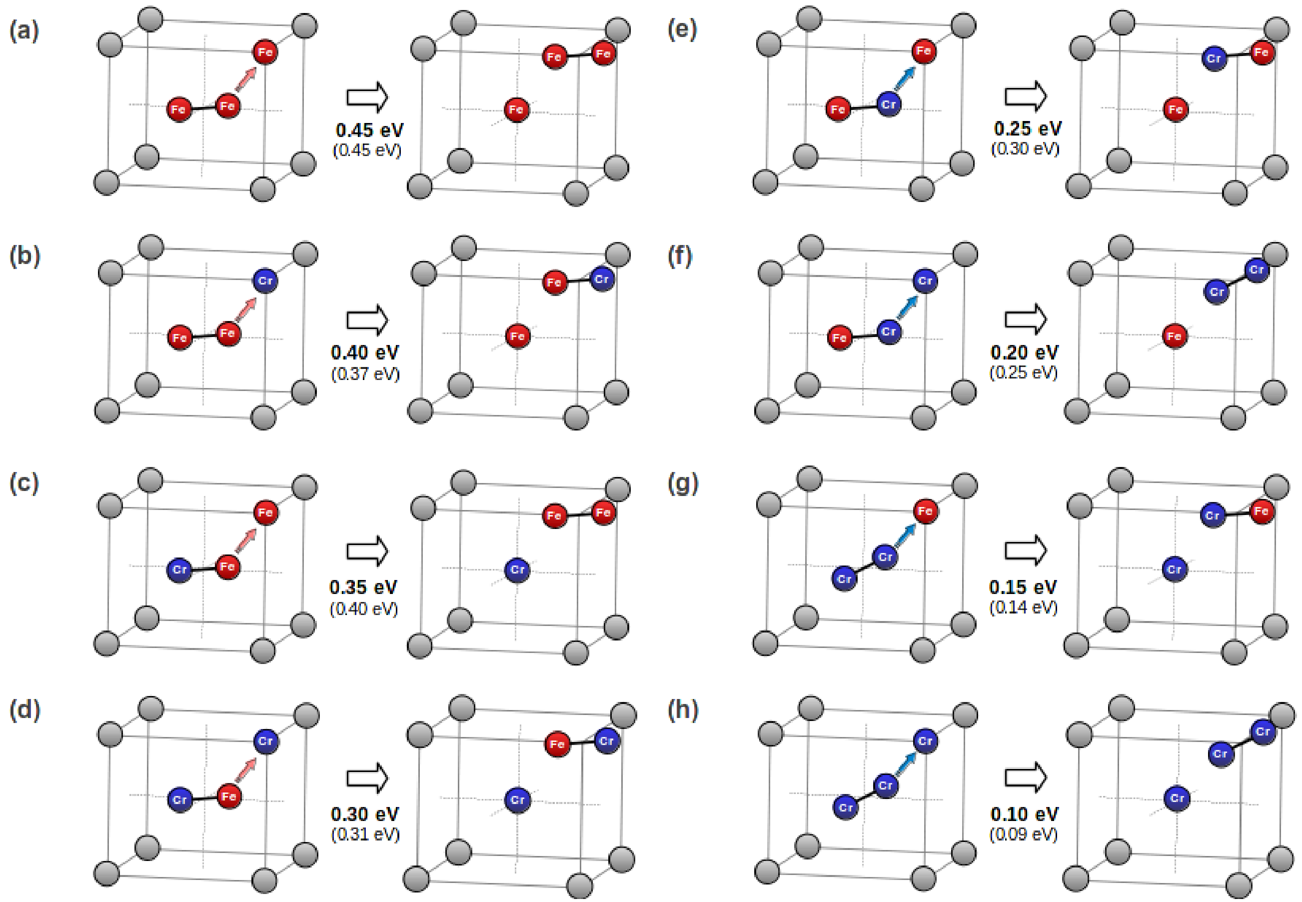
Migration of ICr pairs

- Higher complexity due to migration and particle nature: **FeFe**, **FeCr** and **CrCr** dummbells are considered.
- Formation and break events are implicit in **ICr** migration.

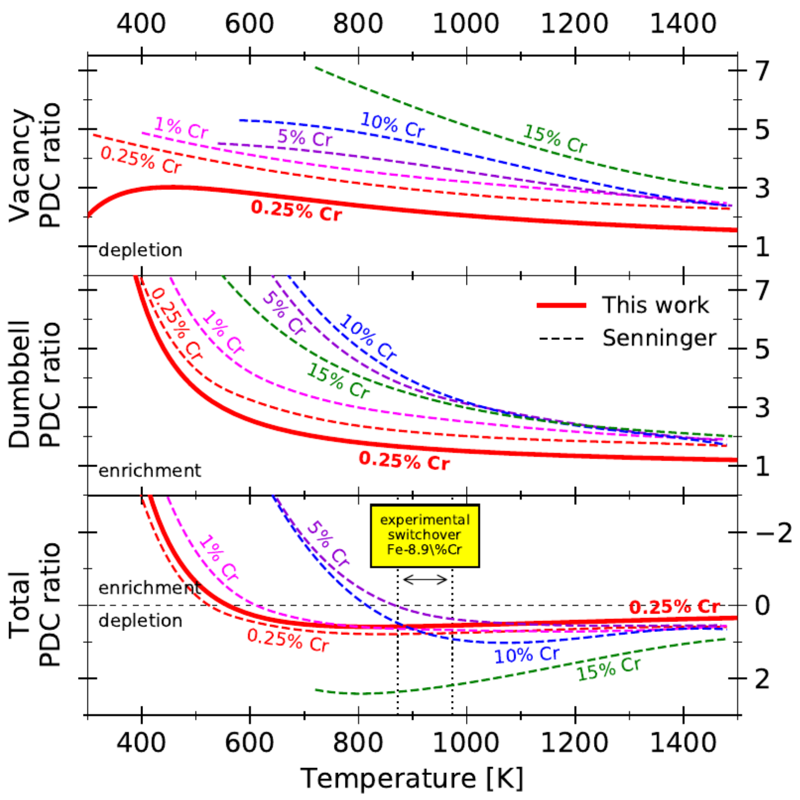
(Id number) The family group of dumbbells transition	*Mean E_{mig} (eV)*	*OKMC E_{mig}(eV)*
(1) (Fe-Fe)+Fe→Fe+(Fe-Fe)	0.45	0.45
(2) (Fe-Fe)+Cr→Fe+(Fe-Cr)	0.37	0.40
(3) (Cr-Fe)+Fe→Cr+(Fe-Fe)	0.40	0.35
(4) (Cr-Fe)+Cr→Cr+(Fe-Cr)	0.31	0.30
(5) (Fe-Cr)+Fe→Fe+(Cr-Fe)	0.30	0.25
(6) (Fe-Cr)+Cr→Fe+(Cr-Cr)	0.25	0.20
(7) (Cr-Cr)+Fe→Cr+(Cr-Fe)	0.14	0.15
(8) (Cr-Cr)+Cr→Cr+(Cr-Cr)	0.09	0.10

Pär Olsson, M4F Plenary Meeting June 2020

Possible migration events due to local configurations:



Self-interstitial assisted migration of Cr

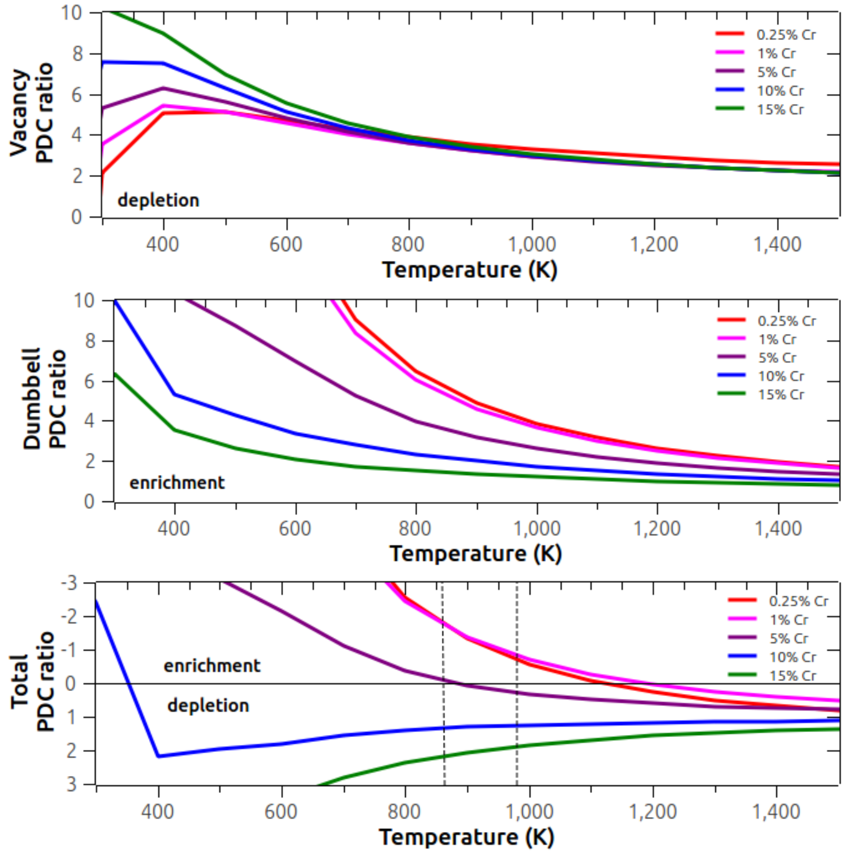


Messina et al, Acta Mat. 191 (2020)

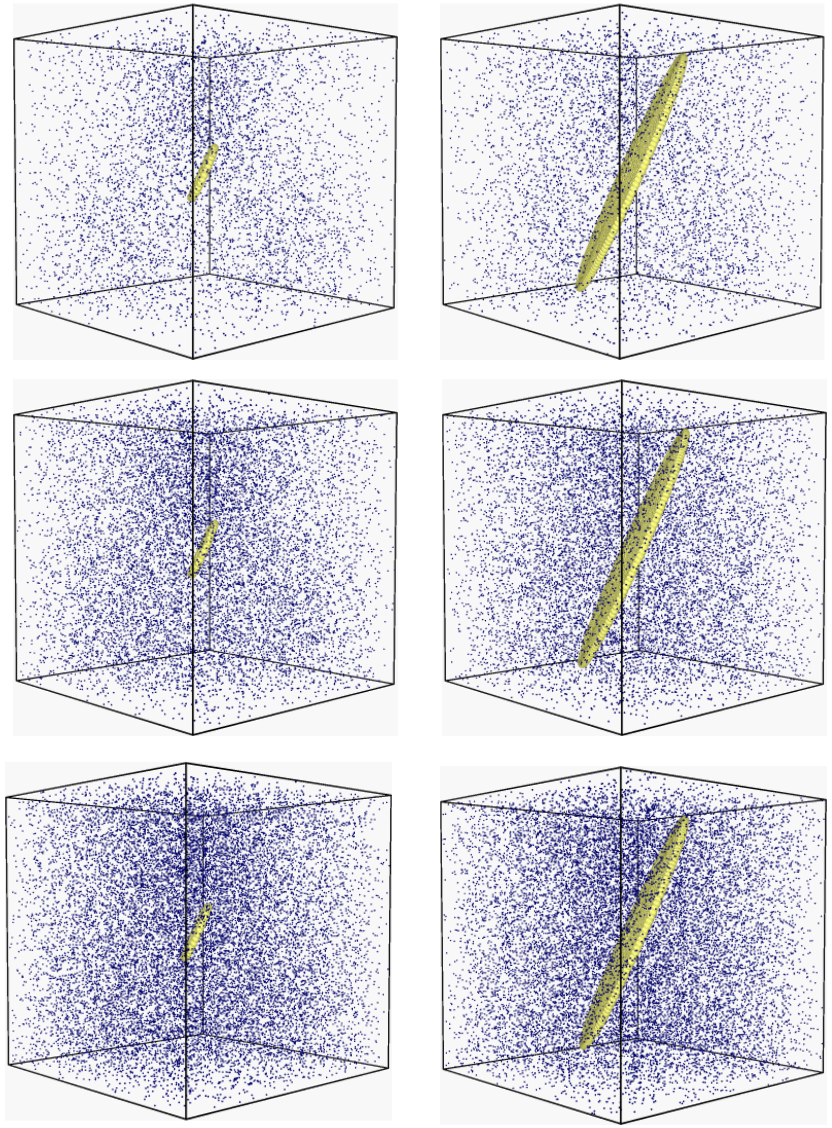
Preliminary results

- Vancacy-mediated migration of solute leads to depletion down to 300K.
- Dumbbell migration predicts enrichment of Cr for any temperature and Cr content.
- Transition from depletion to enrichment for Cr concentrations near 5% around 900 K
- First simulations of dislocation loop decoration with this coarse-grained OKMC model (250 lattice atoms per cell) is not yet able to reproduce enrichment nor depletion.

OKMC simulations



Decoration of dislocation loops

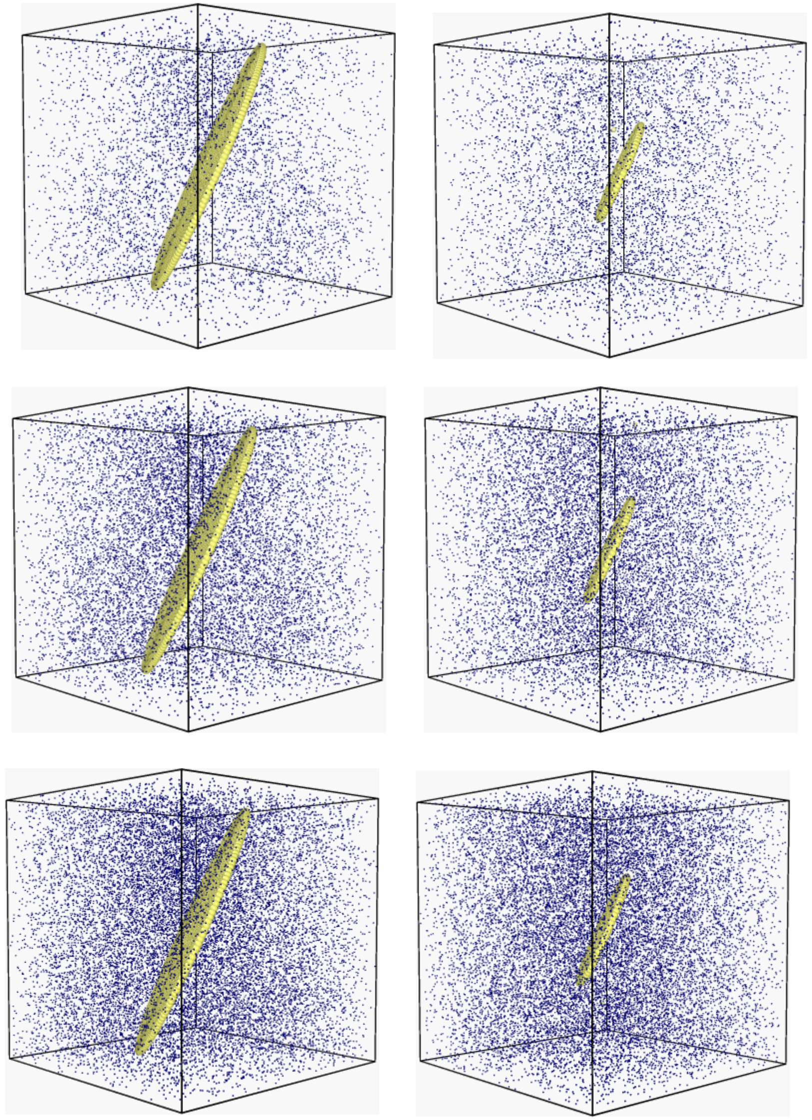


Irradiations with SIA:

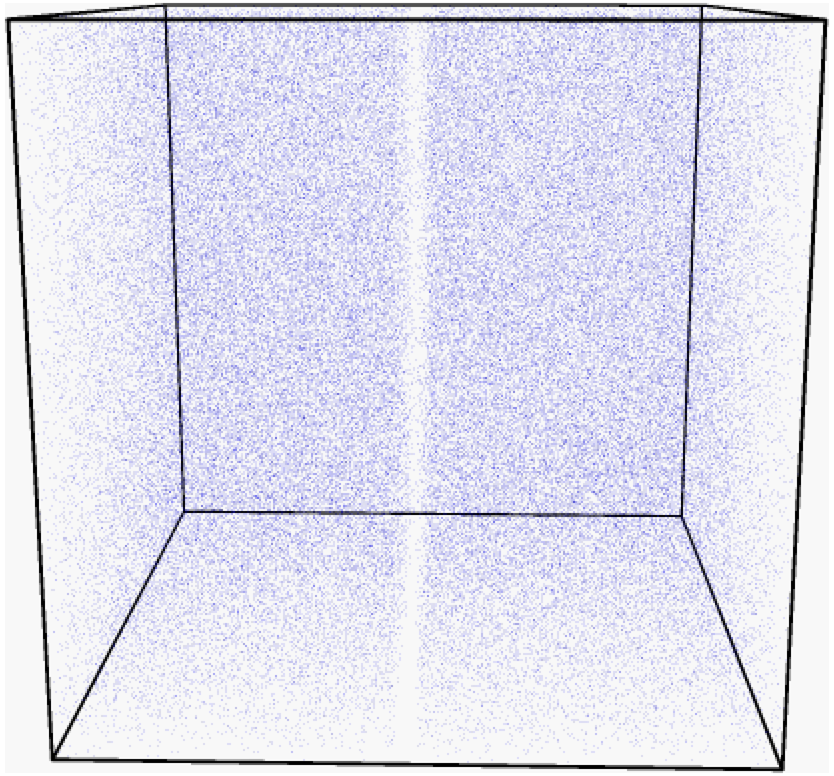
FeCr: 5, 10, 15 and 20%
Volume: 8x8x8 cells (11.48 nm^3)
Cell: $(5\ a_0)^3$, 250 atoms
Temp: 773, 923 and 1073K
Sink: <100> DL (100 SIA)

Irradiations with vacancies:

FeCr: 5, 10, 15 and 20%
Volume: 8x8x8 cells (11.48 nm^3)
Cell: $(5\ a_0)^3$, 250 atoms
Temp: 773, 923 and 1073K
Sink: 100> DL (2000 SIA)



Grain Boundaries

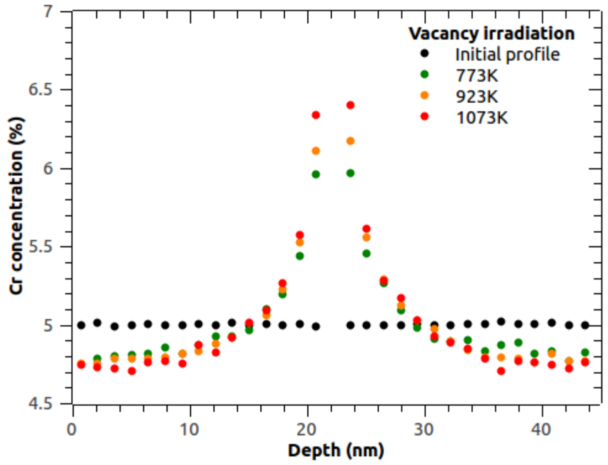


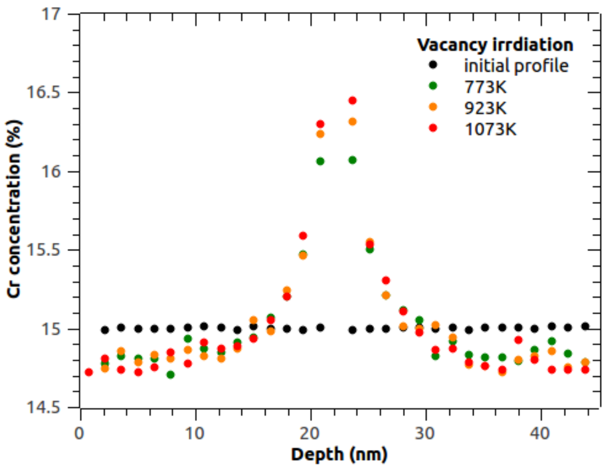
Simulation parameters:

Material:	FeCr alloy
Volume:	32x32x32 cells, $(45.92\ nm)^3$
Cell size:	$(5\ a_0)^3$, 250 atoms
Chromium:	5%, 10%, 15% and 20%
Temperatures:	773K, 923K,1073K
Sink:	empty cells
Cascade:	1 SIA, 1 V and 1 Frenkel pair
Fluence:	1.25e15 $cascades/cm^2$
Flux:	1.00e11 $cascades/cm^2 \cdot s$

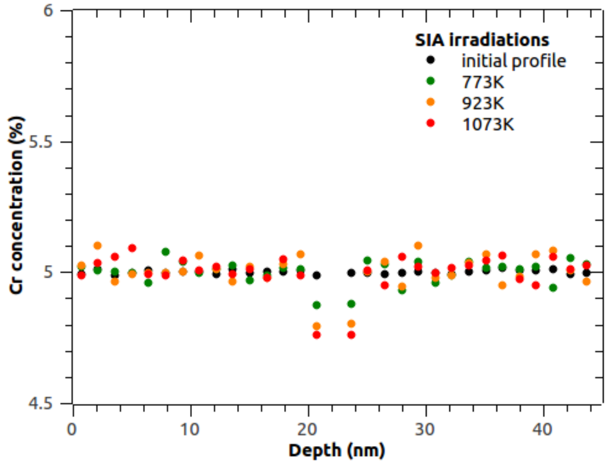
Grain Boundaries

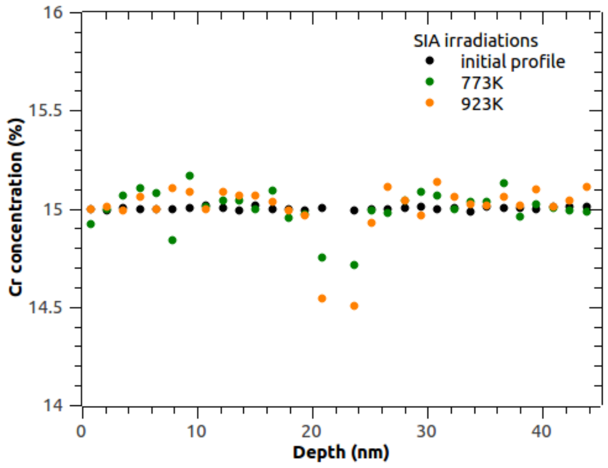
Irradiations with vacancies:



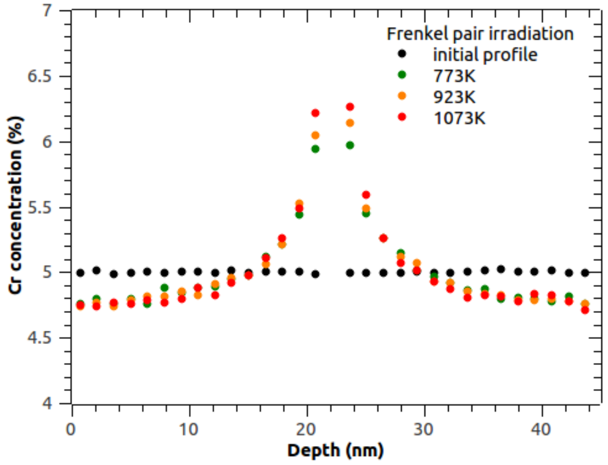


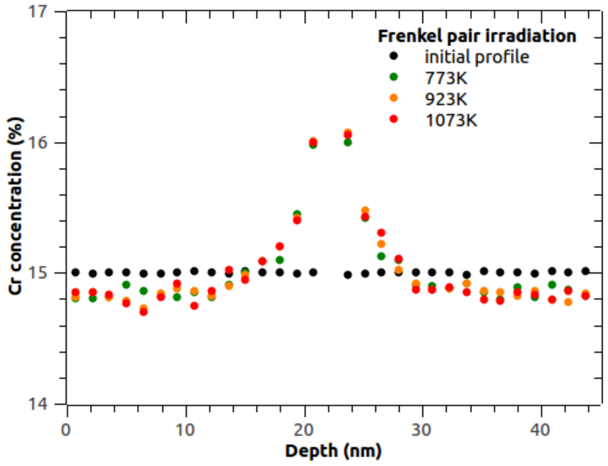
Irradiations with self-interstitials:





Irradiations with Frenkel pairs:





Summary

Summary

1. We have presented a model based on OKMC to reproduce Cr segregation in FeCr alloys.
2. Explicit use of VCr pairs have been used in the vacancy-assisted migration of solute atoms, which successfully reproduced the fomation of Cr precipitates for different cell sizes, L.
3. Implicit use of ICr pairs, as they were treated differently depending of the nature of the 3 involved particles: two of them being part of the dumbbell (FeFe, FeCr, or CrCr) and the third one located at the destination site, where a new dumbbell will be formed.
4. First results of irradiated dislocation loops did not show any noticible decoration with solute atoms.
5. First results of irradiated grain boundaries (GB), modelled as an array of empty cells, did produce Cr enrichment near GB after V irradiation, and Cr depletion near GB after SIA irradiations at the simulated tempteratures.
6. Additional studies are needed.

Acknowledgements

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