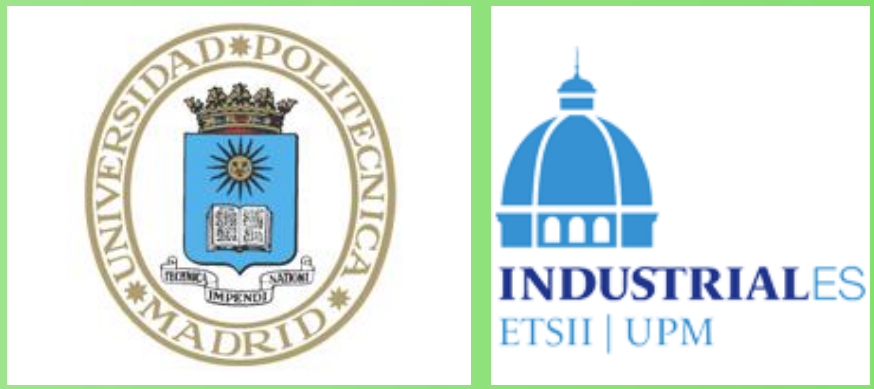


Interstitial defects stability in FeCr alloys vs Cr concentration



E. del Río^{1*}, M.J. Caturla², A. Caro³, M. Serrano³, J.M. Perlado¹

¹ Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Madrid, Spain

² Departamento de Física Aplicada, Universidad de Alicante, Alicante, Spain

³ Materials Science and Technology Division, MST-8, Los Alamos National Laboratory, POB 1663, Los Alamos, NM, USA

Abstract

Finding adequate materials to withstand the demanding conditions in the future fusion and fission reactors is a real challenge in the development of these technologies. Structural materials need to sustain high irradiation doses and temperatures that will change the microstructure over time. A better understanding of the changes produced by the irradiation will allow for a better choice of materials, ensuring a safer and reliable future power plants. High-Cr ferritic/martensitic steels head the list of structural materials due to their high resistance to swelling and corrosion. However, it is well known that these alloys present a problem of embrittlement, which could be caused by the presence of defects created by irradiation as these defects act as obstacles for dislocation motion. Therefore, the mechanical response of these materials will depend on the type of defects created during irradiation. In this work, we address a study of the effect Cr concentration has on single interstitial defect formation energies in FeCr alloys.

Methodology

Molecular static calculations with the interatomic empirical potential specially developed by Alfredo Caro et al. for the study of FeCr alloys based in the concentration dependent model¹. Size cells: 2000 atoms + 1 interstitial atom which could be Fe or Cr. Code: MDCASK.

Results and Discussion

Cr concentration effect:

- Calculations for concentrations of Cr in the range 1 – 17 %
- 2000 calculations for each concentration varying the relative positions of the Cr atoms randomly
- Initial interstitial atoms considered are FeFe and FeCr in three configurations: <100>, <110> and <111>
- The final configuration after optimization has been analyzed to check if it has the same direction and character (FeFe, FeCr) as the original one
- A program was developed to verify the optimised configuration

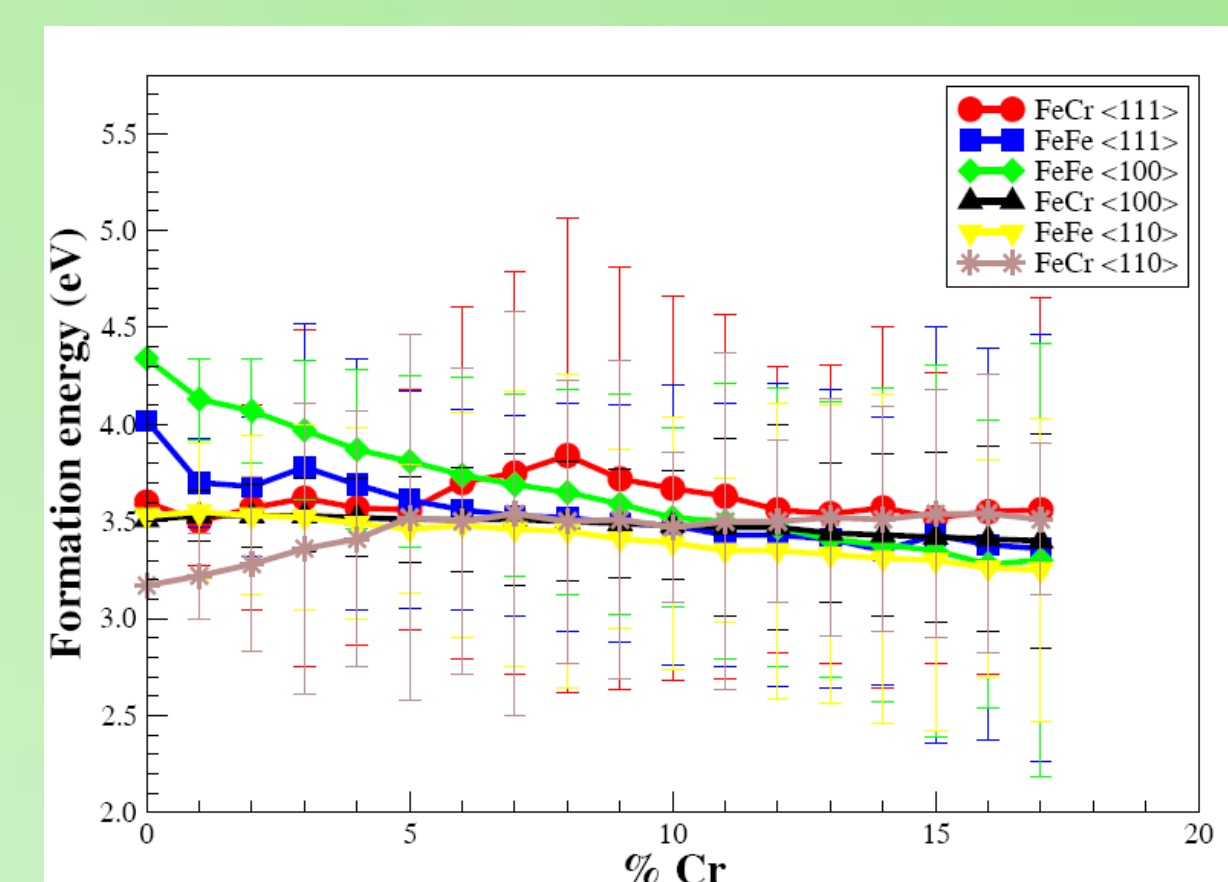


Figure 1. Average formation energy (over 2000 cases) of the different configurations as a function of Cr concentration. All cases included, independently of the final geometry reached after optimization.

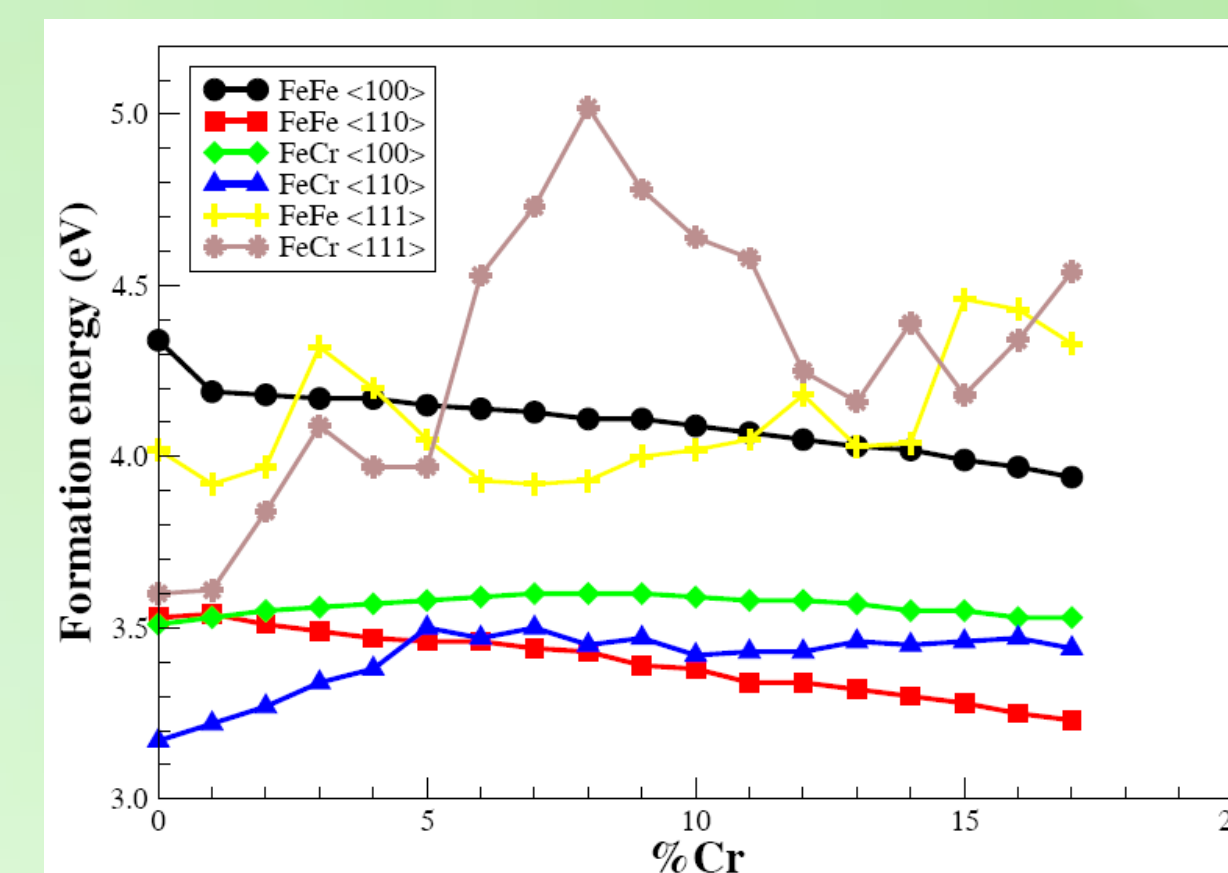


Figure 2. Average formation energy of the different configurations as a function of Cr concentration. Only those cases where the initial and final configurations are the same are considered.

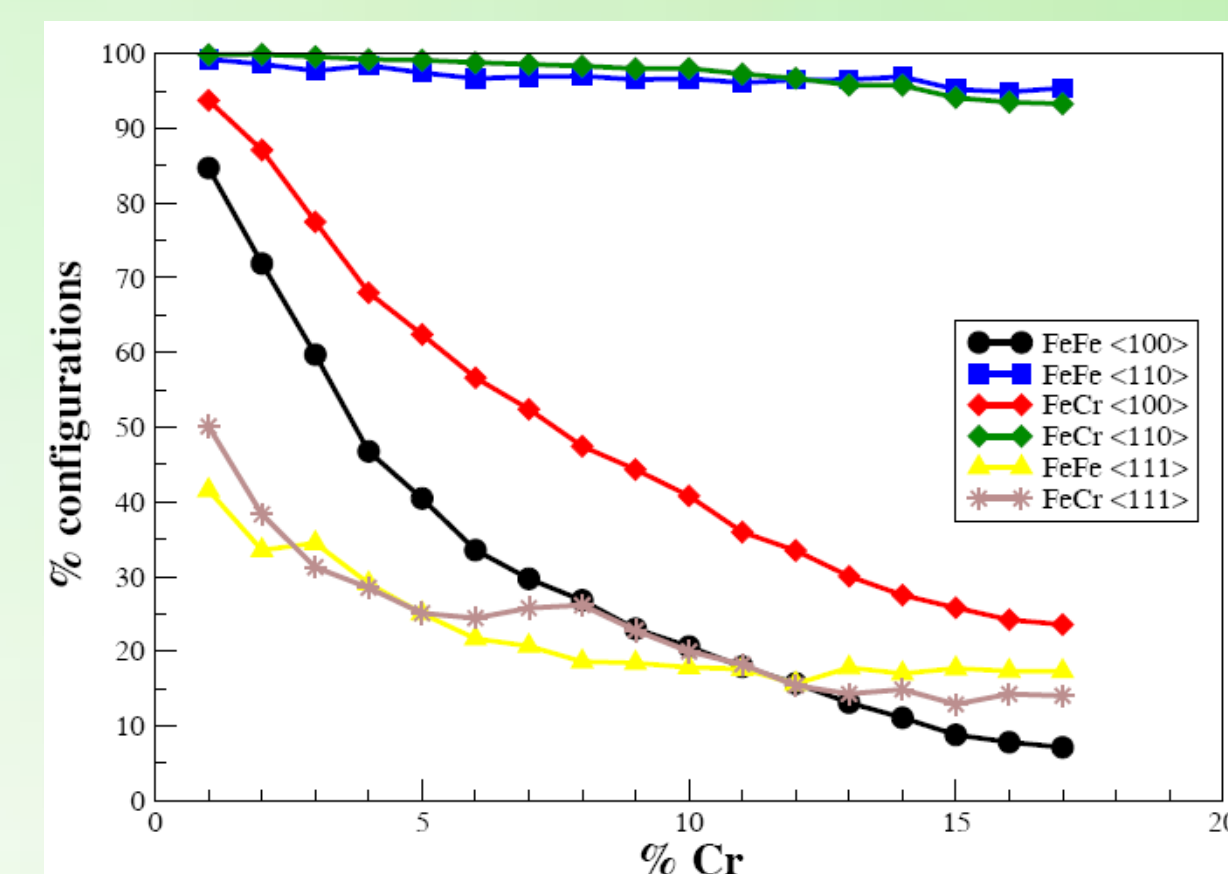


Figure 3. Percentage of configurations that do not change geometry or character used in the calculation of average formation energy of figure 2.

$$E_f = E_{\text{defect}} - (E_{\text{without defect}} + E_{\text{interst}})$$

E_f = Formation energy of the defect

E_{defect} = Energy of the cell with a defect

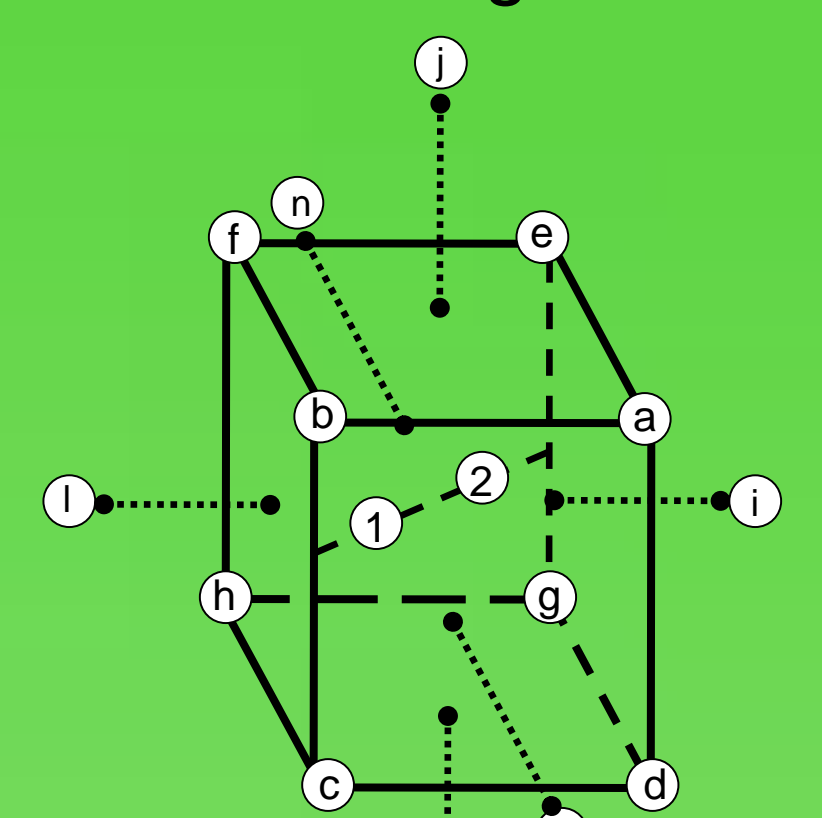
$E_{\text{without defect}}$ = Energy of the cell without a defect

E_{interst} = Energy of the Fe (FeFe interstitial) or Cr (FeCr interstitial) perfect cell per atom

Local Cr distribution effect:

- Calculation of formation energies of FeFe <110> and FeCr <110> when changing the local environment: one Cr atom at different first and second nearest neighbors.

Cr _{subst}	E _f	D ₁₋₂	D _{Cr subst-2}
a, e	3.47	0.740	0.721
c, h	3.47	0.740	1.302
d, g	3.42	0.737	0.927
b, f	3.42	0.737	0.927
i, j	3.49	0.738	0.765
l, m	3.49	0.739	1.328
k, n	3.52	0.733	1.040

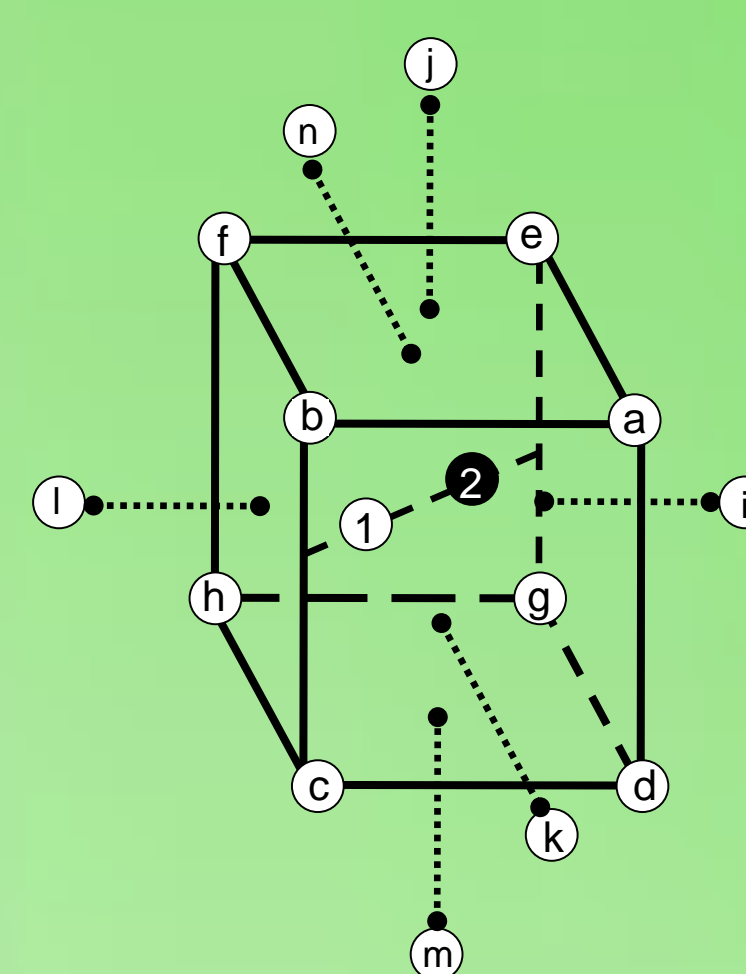


$E_f = 3.53 \text{ eV}$
 $D_{1-2} = 0.736$
 $D_{2-a} = D_{2-e} = 0.763$
 $D_{2-d} = D_{2-g} = 0.923$
 $D_{2-b} = D_{2-f} = 0.923$
 $D_{2-c} = D_{2-h} = 1.318$
 $D_{2-i} = D_{2-j} = 0.817$
 $D_{2-k} = D_{2-n} = 1.054$
 $D_{2-l} = D_{2-m} = 1.323$

○ Fe atoms ● Cr atoms

D_{1-2} = distance between interstitial atoms

$D_{\text{Cr subst-2}}$ = distance between the interstitial atom 2 and the Cr atom at the substitution position, i.e. a, b, c, d, e, f, g, h, i, j, k, l, m, or n



Cr _{subst}	E _f	D ₁₋₂	D _{Cr subst-2}
a, e	3.85	0.709	0.799
c, h	3.16	0.714	1.301
d, g	3.29	0.712	0.958
b, f	3.29	0.712	0.958
i, j	3.44	0.711	0.862
l, m	3.18	0.714	1.338
k, n	3.32	0.711	1.029

$E_f = 3.15 \text{ eV}$

$D_{1-2} = 0.7132$

$D_{2-a} = D_{2-e} = 0.7289$

$D_{2-b} = D_{2-f} = 0.9111$

$D_{2-d} = D_{2-g} = 0.9537$

$D_{2-h} = D_{2-c} = 1.3182$

$D_{2-i} = 0.8449$

$D_{2-j} = 0.7742$

$D_{2-k} = D_{2-n} = 1.0468$

$D_{2-l} = 1.3055$

$D_{2-m} = 1.3545$

Conclusions

- Formation energies converge to a unique value with Cr concentration as can be seen in Figure 1, independently of the starting geometry.
- <110> configurations are the most stable comparing with <100> and <111> configurations
- It is observed a change in the stability of <110> interstitials with Cr concentration:
 - 0 – 5% Cr, FeCr is the most stable
 - 6 – 10% Cr, same stability for self and mixed interstitials
 - 11 – 17% Cr, FeFe is the most stable
- The local Cr distribution study shows that:
 - Formation energy depends strongly on Cr position for the case of FeCr <110> interstitials and weakly in the case of FeFe <110> interstitials.
 - The shorter the distance between Cr atoms, the greater the formation energy

References

[1] a - A. Caro, D.A. Crowson, M. Caro Phys. Rev. Lett.95 (2005) 075702.

b - B. Sadigh, P. Erhart, A. Stukowski, A. Caro. Phil Mag 89 (2009) 3371.

c - E. del Río, J. M Sampedro, H. Dogo, M. J. Caturla, M. Caro, A. Caro and J. M. Perlado. J. Nucl. Mater. 408 (2011) 18-24.

Acknowledgements: This work has been partially supported by the European Commission within the FP7 project GETMAT (Grant agreement number 212175) and FeMAS (FP7-224752), the VI Spanish National Project ENE2008-06403-C06-06 and the European Union Keep in Touch Program on Inertial Confinement Fusion (ref. 08/061) and the European Fusion Development Agreement (EFDA). These results also contribute to the International Atomic Energy Agency CRP SMoRE. AC acknowledges support from the Center for Materials under Irradiation and Mechanical Extremes, a DOE Energy Frontier Research Center.