The Effect of Cr Concentration on Defect Energies in FeCr Alloys

J.M. Sampedro[1], E. del Río[1], M.J. Caturla[2], J.M. Perlado[1]

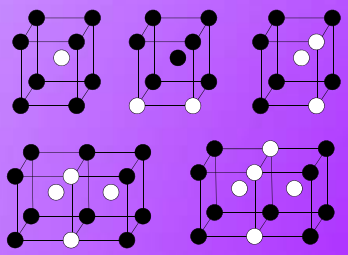
[1] Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Madrid, Spain

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

Abstract: FeCr ferritic alloys are leading candidates for structural applications in generation IV fission reactors due to their high resistance to swelling and corrosion. The addition of Cr improves the behavior of the steels under irradiation, but this improvement is non-monotonic. Understandig the changes in the FeCr ferritic alloys microstructure induced by irradiation and the role played by the alloying element (Cr) is needed in order to predict the response of these materials under the extreme conditions in the future nuclear plants. In this work, we present the effect of Cr concentration in a bcc Fe matrix on binding and formation energies of vacancy clusters.

Method: Molecular static calculations with two different interatomic empirical potentials specially developed for the study of FeCr alloys have been performed in the study of the formation and binding energies of the vacancy clusters. One potential is based on a two-band model formalism (2BM)[1] and the other one has been created introducing an explicit dependence on concentration (CDM)[2]. Initial calculations in order to determine the cluster geometry more stable for each cluster size (up to 5) have been performed over size cells of 2000 atoms. Calculations for the more stable geometries of each cluster size and exploring all the possibilities of the cluster environment were performed on size cells of 250 atoms.

Results and Discussion

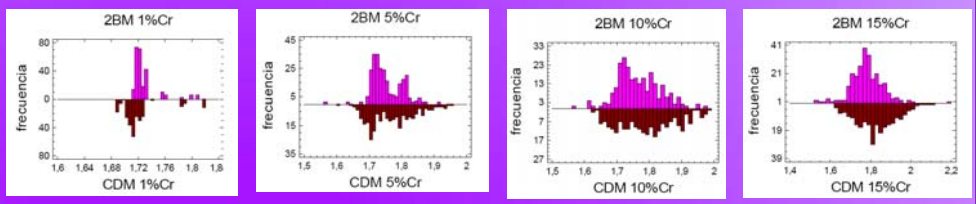


○ Vacancy ● Fe or Cr atoms

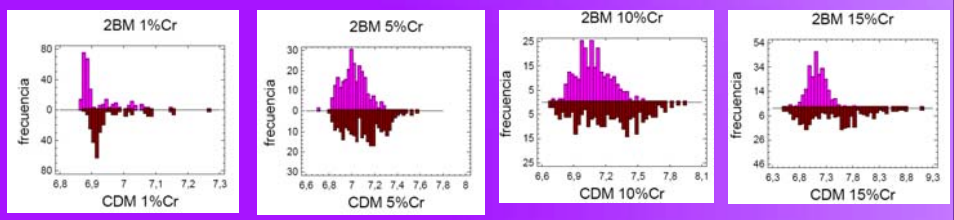
More stable configurations for vacancy clusters

- Only 1nn taken into account except in the case of the divacancy, where the 2nn vacancy cluster is more stable than the 1nn vacancy cluster.

Monovacancy

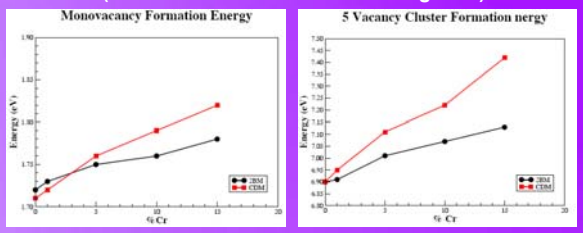


5 Vacancy Cluster



Vacancy cluster formation energy histograms for 1 and 5 vacancies and 1,5,10,15 % Cr for the two interatomic potentials (top 2BM, bottom CDM)

Vacancy cluster formation energy (mean value from the above histograms)



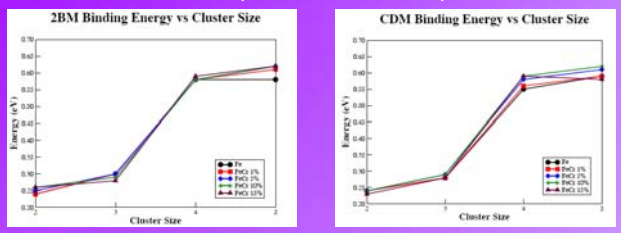
$$E_f = E_{defect} - (E_{without\ defect} - n_{Fe}\,E_{Fe} - n_{Cr}\,E_{Cr} - \Delta h)$$

E_f = Formation energy of the defect
E_{defect} = Energy of the cell with a defect
$E_{without\ defect}$ = Energy of the cell without a defect
n_{Fe}, n_{Cr} = Number of Fe or Cr atoms removed, respectively
E_{Fe} = Energy of the Fe perfect cell per atom
E_{Cr} = Energy of the Cr perfect cell per atom
Δh = Enthalpy difference between initial and final % Cr

- Higher Cr concentrations or cluster size provide more possibilities of having Cr at 1nn or 2nn positions ⇒ Greater dispersion of values in the formation energy between different configurations for the same cluster size and Cr concentration.
- Higher dispersion for the CDM potential.

- Formation energy increases with:
  - The cluster size
  - The Cr concentration
- CDM potential predicts higher formation energies than the 2BM potential.
- These differences are greater for higher Cr concentrations

Binding energy of a single vacancy to a cluster of size n (n from 2 to 5 defects)



$$E_{a-b} = E_a + E_b - E_{ab}$$

E_{a-b} = Binding energy between defect b and 1 vacancy
E_a = Monovacancy formation energy
E_b = (n-1) Vacancy cluster formation energy
E_{ab} = n Vacancy cluster formation energy

- Similar energies with CDM and 2BM potentials
- Same energy values for Fe or FeCr alloys with 1,5,10,15% Cr
- Energy increases with the cluster size
- Small increases in the binding energy for 3 and 5 vacancy clusters with respect to the 2 and 4 vacancy clusters respectively
- Great increase in the binding energy for 4 vacancy clusters from 3 vacancy clusters

Conclusions

-CDM potential more sensitive to the Cr local concentration
-Similar results for the vacancy cluster formation energy for both potentials studied
-Differences in the formation energy between CDM and 2BM potentials more appreciable with:
  - the Cr concentration
  - the size of the cluster
-Stability increases with the cluster size for vacancy clusters up to 5
-Binding energy does not depend on the Cr concentration for both potentials.

Further work

- Study the effect of the Cr concentration on:
  - 111, 110 and 100 FeFe and FeCr Interstitials Formation Energy
  - Formation and Binding energies of Interstitial Clusters
- Study the effect of the Cr local concentration on the Interstitial Formation Energies
- Study the mobility of the interstitial in the FeCr alloy

References

[1] P. Olsson, J. Wallenius, C. Domain, K. Nordlund, L. Malerba, Phys. Rev. B 72 (2005) 214119.

[2] 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 Rio, J. M Sampedro, H. Dogo, M. J. Caturla, M. Caro, A. Caro and J. M. Perlado. J. Nucl. Mater. (2010), doi: 10.1016/j.nucmat.2010.10.021

Acknowledgements: We want to thank Alfredo Caro and Lorenzo Malerba for useful discussions. 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.