The Effect of Cr Concentration on Defect Energies in FeCr Alloys

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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. Understanding 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)² 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 cluster formation energy (mean value from the above histograms)

- 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

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.

References


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