



Defect energetics in FeCr from empirical interatomic potentials



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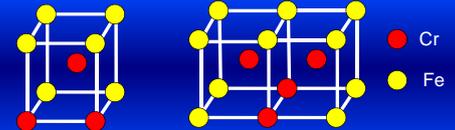
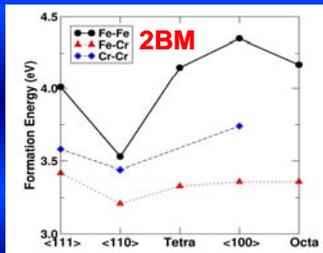
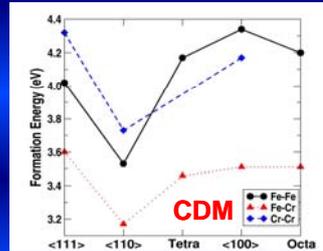
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Abstract: We present a comparative study between two empirical potentials for the study of FeCr alloys. Vacancy, self- and mixed interstitials formation energies are investigated for both potentials in pure bcc Fe and pure bcc Cr. These results are compared to DFT values reported in literature. Some small Cr clusters in substitutional positions have also been studied in bcc Fe. Finally we have performed some calculations of the vacancy formation energy (E_v) depending on Cr concentration.

Method: Molecular static calculations with two different interatomic empirical potentials specially developed for the study of FeCr alloys. One is based on a two-band model formalism (2BM) and the other one has been created introducing an explicit dependence on concentration (CDM). Size cell calculations: 2000 atoms

Point defect formation energies

- Substitution energy of Cr in bcc Fe: -0.29 eV (2BM), -0.14 eV (CDM), -0.12 eV (DFT)
- Fe-Fe potential and Cr-Cr potential are the same for 2BM and CDM potentials.
- Formation energies of the vacancy and self-interstitials in pure bcc Fe and pure bcc Cr are the same for both potentials
- Cr-Cr $\langle 110 \rangle$ dumbbell is the most stable configuration in pure bcc Cr
- Self-interstitial formation energies in pure bcc Cr more than 1 eV larger than those in pure bcc Fe
- $\langle 110 \rangle$ dumbbell is the most stable configuration for Fe-Fe, Fe-Cr and Cr-Cr in pure bcc Fe
- Same stability order of the formation energies of Fe-Cr interstitials for both potentials
- $E_{\text{Fe-Cr } \langle 111 \rangle} - E_{\text{Fe-Cr } \langle 110 \rangle} = 0.21 \text{ eV (2BM), } 0.43 \text{ eV (CDM), } 0.41 \text{ eV (DFT)}$
- Both potentials reduce the energy differences between the configurations when comparing Fe-Cr with Fe-Fe interstitials



Cr+Cr+Cr (triangle) Cr+Cr+Cr+Cr (tetrahedral)

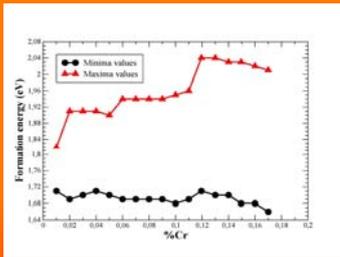
Configuration	CDM Formation energy (2000 atoms)	2BM Formation energy (2000 atoms)	PAW ^a (128 atoms)
V-Cr 1nn	1.64	1.53	1.98
V-Cr 2nn	1.67	1.57	2.02
V-Cr 3nn	1.54	1.49	
V-Cr 5nn	1.56	1.49	
Cr + Cr 1nn	0.09	-0.26	0.02
Cr + Cr 2nn	-0.03	-0.27	-0.01
Cr + Cr 3nn	-0.22	-0.29	
Cr + Cr 5nn	-0.27	-0.41	
Cr + Cr + Cr (triangle)	0.37	-0.27	0.15
Cr + Cr + Cr + Cr (tetrahedral)	0.72	-0.31	0.27

V-Cr: good agreement between both potentials and DFT
Cr clusters: energy almost constant with the number of Cr-Cr pairs for 2BM whereas it increases for DFT and CDM

Formation energies of Cr clusters

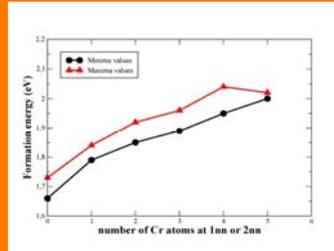
Cr concentration effect on E_v

- Calculations have been performed with:
 - the CDM potential and Cr concentrations from 1% to 17%



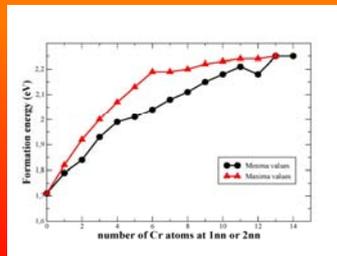
Dependence of E_v on Cr concentration and distribution

- 4 different distributions studied
- The minimum value is almost constant with increasing Cr concentration
- The maximum value rises as the Cr concentration increases



Dependence of E_v on the number of Cr atoms considering different Cr concentrations but assuming that relevant Cr atoms are only located at 1 or 2 nearest neighbor (nn)

- The energy increases when a new Cr atom is introduced at 1nn or 2nn position.



Dependence of E_v on the number of Cr atoms selecting the Cr concentration as the Cr atoms can only be located at 1nn or 2nn.

- Maximum number of Cr atoms: 14
- The E_v increases:
 - from 1.71 eV (E_v in pure bcc Fe) to 2.25 eV (E_v in pure bcc Cr 2.56 eV)

Conclusions

- Fe-Cr interstitials more stable than Fe-Fe and Cr-Cr interstitials.
- Tetrahedral and octahedral configurations stabilized with respect to the $\langle 111 \rangle$ dumbbell, in contrast with DFT for Fe-Cr interstitials.
- Different order of stability of $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ configurations for Cr-Cr interstitials:
 - 2BM: same order of stability than DFT but Cr-Cr interstitials more stable than the Fe-Fe ones
 - CDM: correct ordering for the different $\langle 110 \rangle$ dumbbells. It does not reproduce the stabilities of the $\langle 111 \rangle$ and $\langle 100 \rangle$ interstitials
- E_v increases when the Cr atoms are located in the 1 or 2 nn position. Cr atoms placed in other lattice sites might not significantly affect it.

Further work

Study the effect of the Cr concentration on:

- Interstitials formation energy
- Vacancy cluster, formation and binding energy
- Interstitial cluster, formation and binding energy