Materials Science Forum Vols. 706-709 (2012) pp 1095-1099
Online available since 2012/Jan/03 at www.scientific.net

doi:10.4028/www.scientific.net/MSF.706-709.1095

Density Functional Theory and ab initio molecular dynamics study of the effect of Ti and Zr transition metals in $D0_3$ Fe_3Al

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Keywords: Fe_3Al-$D0_3$, transition metal, ab initio, grain boundary, defect stability.

Abstract

The formation energies of the T.M impurities Ti and Zr were calculated using DFT calculations at absolute zero and ab initio MD simulations at 300 K. We found that, with increasing temperature, Zr impurities become more stable and prefer to segregate at the interface of ∑5 (310)[001] grain boundary. In the case of Ti, the results show that it remains a stable defect when temperature increases.

Introduction

Fe_3Al-based alloys have been studied widely as candidates for high-temperature structural applications [1–2]. Their main advantages are the excellent high-temperature corrosion resistance in oxidizing and sulfidizing environments and their low density. However, because of their limited room temperature ductility and their low strength and creep resistance at higher temperatures, it is necessary to improve their properties to adapt them for structural applications. The addition of ternary alloying elements of transition metals (T.M.) can be used with the objective of increasing the $D0_3$-B2 transition temperature (T_0) [3-4]. The efficiency in raising T_0 $^{D03\text{-}B2}$ varies strongly for the different solutes. Whereas Zr addition has limited effect, the addition of Ti results in a particularly large increase of T_0 $^{D03\text{-}B2}$ of about 60 K/at.% [3-4]. The effect of T.M. solute on T_0 is expected to be related to its crystallographic site preference of the T.M. atoms in the $D0_3$ structure. Transition metals such as Ti [3, 5], V [4], Cr[6] and Mo[3] are known to occupy the FeI sites (4(b) sites in Wyckoff notation) of the $D0_3$-ordered structure of Fe_3Al . However, the situation is less clear concerning an element such as Zr for which there is no data on site preference in $D0_3$-Fe_3Al. In the present work we performed DFT calculations at absolute zero and ab initio molecular dynamics (MD) at 300 K to compare the behavior of Zr and Ti alloying elements both within the bulk and at grain boundaries. The temperature dependence stabilities of these two T.M are also discussed.

Computational methods

The DFT calculations at 0K and ab initio molecular dynamic MD simulations at 300 K were performed using the Generalized Gradient Approximation formulated by Perdew-Wang functional (GGA-PW91) [7] and the UltraSoft PseudoPotential (USPP) method [8], as implemented in the