First principle study of the effect of Ti and Zr transition metals located in bulk D0(3)Fe(3)Al and Sigma 5 (310)[001] grain boundary

Auteur: Chentouf, S; Raulot, J. -M.; Aourag, H.; Grosdidier, T.

Abstract/Résumé : The effects of Ti and Zr transition metal impurities located in the bulk as well as at the Sigma 5 (310)[001] tilt grain boundary in an ordered (D0(3)-Fe3Al) intermetallic were studied by means of ab-initio calculations. In the bulk, FeII sites are the preferential sites for vacancies while Ti and Zr prefer to reside on FeI sites. The interface energy of a clean Sigma 5 (310) interface has been found to be (0.36 J/m(2)). The lowest formation energies for the T.M. substitutions have always been obtained on FeI sites on the first plane away from the exact grain boundary interface. Ti and Zr impurities are found to reduce the interface energies on various sites of this Sigma 5 (310) grain boundary by an average of 14% and 22%, respectively. However, significant differences between the behavior of Zr and Ti atoms were revealed. Ti is within the bulk, while, comparatively, Zr is stable within the grain boundary both as an insertion (with Fe first neighbors) and as a substituting element (on FeI and FeII sites). Also, the creation of FeII vacancies in a Ti-doped boundary is energetically costly while it is favored in a Zr-doped one.

Keywords/Mots cléfs : Ab-initio calculations; Elastic properties; Intermetallic compounds

Journal title / Revue INTERMETALLICS

,0966,9795,"DOI"10.1016/j.intermet.2012.03.032

, ?, "issue" ,1 , "volume" , 28

0 , "pp" 1 ;10,

sept-12

WOS:000307038700001

Source: