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Physical properties investigation of $Fe_{1-x}Al_x$ ($x \leqslant 50$%-at) alloys using DFT and Wagner-Schottky model

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Abstract

Atomistic modeling based on the Density Functional Theory (DFT) is used to study the structural, magnetic, electronic and mechanical properties of $Fe_{1-x}Al_x$ alloys ($x \leqslant 50$%-at) with and without B, C and N additions over the selected range of Al atomic concentration. It is shown that a singularity around $x_{Al} \sim 40$%-at is observed for the lattice parameters while the magnetic moment decreases uniformly without unexpected trend. The enthalpies of formation indicate that the presence of B stabilizes the system for Al concentration in the range of 25%-at $< x_{Al} <$ 45%-at and the electronic properties are affected by B, C and N additions. The trends in Young modulus, bulk modulus, expected ductility (Pugh ratio) and Vickers hardness evolution are also estimated. N addition improves the Young modulus of alloy while C addition increases its ductility. By using the Wagner-Schottky model, temperature and composition dependences of thermal vacancies in B2-FeAl reveal that the double defect Al^{Fe} anti-sites and Fe vacancies are dominating in the Al-rich side at finite temperature. In addition, the diffusion phenomenon is observed for B, C and N atomic defects.

Keywords: iron aluminides, magnetic properties, elastics proprieties, electronic structures, DFT calculations, thermal defects, Wagner-Schottky model

(Some figures may appear in colour only in the online journal)

1. Introduction

Iron-aluminides are considered as potential candidates for medium and high temperature applications in a wide range of mechanical and magnetic industries [1, 2]. They present an excellent resistance to oxidation and corrosion, low densities, high melting points, good mechanical properties at high temperatures and a low raw material cost [3–6]. It is well-known that their alloying, mechanical properties, hardening processes, transport and diffusion phenomena are highly sensitive to the type and concentration of defects (e.g., thermal vacancies) as well as the deviation from the stoichiometry [7–11]. In the iron-rich side of the FeAl system, the body-centered cubic (*bcc*) phases with B2 (CsCl-type) as well as DO3 (BiF_3-type) structures are stable over a large range [12]. Several theoretical and experimental studies have investigated the effect of ternary additions on the mechanical properties of FeAl alloys with Al content [12–18]. Experimentally, Y Liu *et al* [19] showed that FeAl is hard with strong anisotropy. M R Harmouche *et al* [17] demonstrated similar composition dependences with modulus clustering near 260 GPa for FeAl at room temperature. J Liu *et al* [20] studied the thermal stability and thermal shock resistance of the Fe_2AlB_2 at high temperatures. They found that the strength of the quenched

