Electronic Structure and Magnetism of Alloying Elements Substituted B2 FeAl Intermetallic Compounds: A Density Functional Study

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1. Introduction

The iron aluminides based on Fe_3Al ($D0_3$-type) and FeAl (B2-type) intermetallic compounds have been the subject of intense study due to their potential technological and industrial applications. In particular, the B2 ordered Fe-Al intermetallic compounds are being investigated since their intriguing properties such as, low density, good corrosion resistance, good thermal conductivity, and low material cost, and so on. Moreover, these materials have excellent soft magnetic properties. However, it is known that these systems have low ductility and brittle fracture toughness at ambient temperatures. In order to improve their mechanical and magnetic properties, recently several studies are in progress on alloying element additions into Fe-Al alloys, but few investigations are presented [1]. Therefore, there is a need for a systematic first-principles study on fundamental thermodynamic and magnetic properties of transition metal (TM) substituted B2 ordered FeAl intermetallic compounds. In this work, we used the all-electron full-potential linearized augmented plane wave (FLAPW) method [2], well known for its most suitable in magnetic system calculation.

2. Computational Model and Method

In the present calculations, we used the various alloying elements (3*d* and 4*d* TMs) substituted 2×2×2 supercell (contained 16 atoms) of the B2-FeAl structure. This composition corresponds to a alloying element content of 6.25 at.%. In order to find preferential site stability, we consider the alloying element substitute into a Fe or Al site. Note that there are only two nonequivalent sites (denoted as Fe- or Al-site). In the FLAPW calculation, the generalized gradient approximation (GGA) [3] for the exchange correlation potential was used. An energy cutoff of 4.5 ($2\pi/a$), where a is the lattice parameter, was employed for expanding the linearized augmented plane wave basis set. An 18.0 ($2\pi/a$) star function cutoff was used for depicting the charge density and potential in the interstitial regions. Lattice harmonics with $l \leq 12$ were employed to expand the charge density, potential, and wave functions inside each muffin-tin sphere. Integrations inside the Brillouin zone (BZ) were performed using the improved tetrahedron method over a 13×13×13 mesh within the three-dimensional (3D) BZ.

3. Results

In order to determine preferential site occupations of alloying elements in the B2 FeAl, we calculated the formation enthalpy ΔH, which also can be understood as the relative stability. As a result, it was shown that the

early 3*d* and 4*d* TMs would occupy Al-site, whereas the late 3*d* TMs would occupy Fe-site, from the formation enthalpy calculation. In addition, we found out that the formation enthalpy of Ti, V, Co, Ni, Zr, and Nb substituted Fe-Al systems are lower than that of binary B2 FeAl. This means that these elements show good solubility in B2 ordered Fe-Al system. On the other hand, Cr, Mn, Cu, Zn, and Mo elements seem to disturb forming of B2 ordering.

In Table I, we list calculated spin magnetic moments for 3*d* and 4*d* TMs substituted B2 FeAl. In the Cu substituted system, it is interesting to find out that even though the starting spin configuration is set to a ferromagnetic, the self-consistent calculation is converged to the nonmagnetic state. Moreover, the Sc substituted system has the highest total magnetic moment.

Table I. The calculated spin magnetic moments (in units of μB)

TM	Stable Site	Magnetic Moments			
		TM	Fe atom	Al atom	Total
Sc	Al	-0.122	0.845	-0.039	6.233
Ti	Al	-0.211	0.708	-0.029	5.117
V	Al	-0.292	0.583	-0.022	4.122
Cr	Al	-0.339	0.456	-0.015	3.109
Mn	Al	1.968	0.557	-0.030	6.192
Fe	-	-	0.771	-0.031	5.869
Co	Fe	0.040	-0.601	0.027	-4.690
Ni	Fe	0.061	0.634	-0.027	4.429
Cu	Fe	0.000	0.000	0.000	0.000
Zn	Fe	0.296	-1.205	0.009	-3.060
Zr	Al	-0.139	0.710	-0.034	5.169
Nb	Al	0.142	-0.557	0.024	-4.060
Mo	Al	-0.128	0.412	-0.017	2.982

4. Summary

In this study, the thermodynamic and magnetic properties of alloying element substituted B2 FeAl systems have been investigated using the all-electron FLAPW method based on the GGA. It was shown that the important changes take place in the structural properties as well as in the magnetism when alloying element is substituted by Fe or Al site in B2 FeAl. Detailed discussion on the thermodynamic and magnetic properties and electronic structure of these intermetallic compounds will be given.

5. References

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