A study on Binary Alloy Bethe Model with B2 FeAl

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1. Introduction

Alloy consists of several kinds of atoms which make up superlattice order, and this superlattice order breaks down as atoms agitate thermally with increasing temperature. This characteristic makes difficult to study alloy systems, due to its complexity of considering randomness of their configurations. The simplest approximation is the Bragg-Williams approximation [1] which models alloy system similar to the Ising model, within the mean-field theory. It calculates the energy of the system from the interchange energy between different atoms proportional to the order parameter of the system. Another one is the Bethe approximation [2], which utilizes the partition function involving the short-range interactions between atoms, and also considers the long-range interactions. In the previous study, the analytic and numerical result of Bethe approximation for quadratic lattice was given [3].

In the present work, the analytic solutions to the Bethe approximation for body-centered cubic lattice are worked out and applied to the B2 FeAl intermetallic alloy. The interaction parameters Fe and Al atoms were obtained from the density functional calculations. Moreover, the results are to be compared with experimental values, in order to find the relationship between the atomic disorder and the magnetism of the alloy.

2. Calculation models

Fig. 1 shows how the Bethe's second approximation works. We choose, in the atomic lattice, an arbitrary atom as a central atom, and consider the configurations of its surrounding atoms, called as “shell”s. In the Fig. 1, the crossed circle is the central atom. The squares surrounding it are the nearest neighbor atoms of the central atom, which are called as the “first shell”, and the crosses and the circles surrounding the first shell are called as the “second shell”, and so on. While the first approximation only utilizes the configuration of the central atom and the first shell, and consider the outer shells as a effective field, the second approximation also uses the configurations of the second shell, which makes the approximation much more realistic.

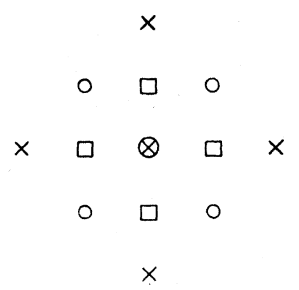

Figure 1. Bethe's approximation in the quadratic lattice [2].

By this approach, the partition function of the system is obtained, and from the partition function the following thermodynamic functions can be calculated (see Ref. 3)

$$F = -\frac{1}{\beta}\ln Z,\quad U = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{N,V},\quad S = \frac{-F+U}{T},\quad C = \left(\frac{\partial U}{\partial T}\right)_{N,V} \quad (5)$$

3. The Relationship between the Atomic Disorder and Magnetism in B2 FeAl Intermetallic

As many literatures indicate, the Density Functional Theory (DFT) calculation shows that the B2 FeAl intermetallic compound is ferromagnetic in ground state with Fe atom's magnetic moment $\cong 0.7\mu_B$, while it is paramagnetic at room temperature [4-6]. In this work, we assume that FeAl has ferromagnetic-paramagnetic transition, and also assume that this magnetic transition is closely related to the atomic order-disorder transition, simply as one-to-one correspondence. Thus, we obtain the atomic interation energy between Fe and Al in FeAl from DFT calculations, apply it on Bethe approximation to model the atomic disorder, and observe how the change of magnetism is related to the atomic disorder of FeAl, comparing with the existing experimental results.

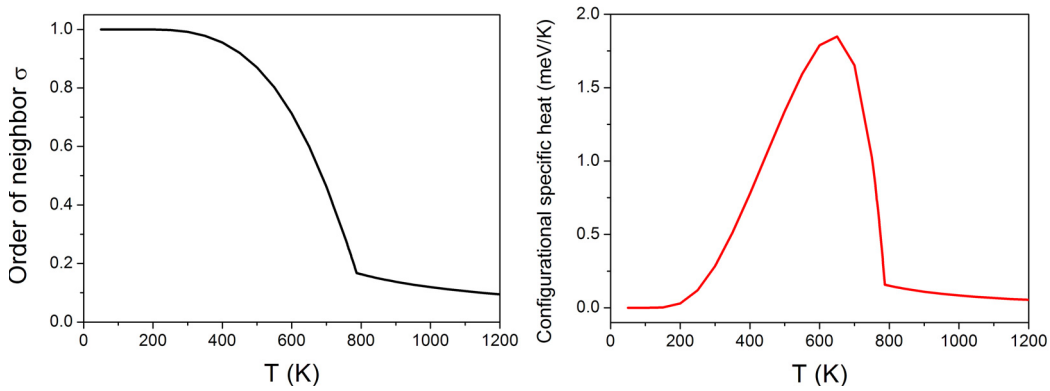

Figure. 2. The order-disorder transition of BCC (B2) alloy modelled by the Bethe approximation, for the case when the interaction energy between different atoms is 20 meV.

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