On the Ising Characteristic of Bragg-Williams and Bethe Alloy Models

Jee Yong Lee*, Won Seok Yun, In Gee Kim
Graduate Institute of Ferrous Technology, Pohang University of Science and Technology,
Pohang 790-784, Republic of Korea

Corresponding Author: igkim@postech.ac.kr

1. Introduction

The study on order-disorder transition of alloy has been done for a long time. However, it mostly relies on only a few physical models, such as the Bragg-Williams model [1-3] which is similar to the Ising model of ferromagnetism with the mean field approximation, and the Bethe model [4] which is a extension of the Bragg-Williams model. These models need some parameters, and the CALPHAD method, which relies on the Bragg-Williams model to calculate phase diagrams of alloys, uses the experimental data for parameters [5].

Firstly, we intended the use of experimental data of alloy model to be replaced by the computational data from the first-principles calculations, to result in a more accurate simulation of the order-disorder transition of the alloy system, without experiments. Moreover, we have observed the alloy models with respect to the general Ising model, and have made various attempts to obtain characteristics of the models.

2. Calculation models

At equilibrium the free energy derivative with respect to the order parameter ϕ should be zero: $\frac{\partial S}{\partial \phi} = T^{-1}\frac{\partial U}{\partial \phi}$. The Bragg-Williams model for binary alloy uses some assumptions:

1. All the α-positions (A-atom reservoir) are identical and all the β-positions (B-atom reservoir) are identical.
2. The interchange of an A atom in an α-position with a B atoms in a β-position means a unique increase in Δ in internal energy.
3. The internal energy U associated with the atomic arrangement a unique function of ϕ.

$$\Delta(\phi) = -\frac{1}{[rn(q-a)]}\frac{\partial U(\phi)}{\partial \phi}$$

where n, a, r are parameters represent the total number of atoms, the fraction of A atoms, and the fraction of α-sites, respectively. Also, q is the maximum value of probability p for an A atom to occupy at an α-sites.

Then the equilibrium condition is

$$f_1(\phi) \equiv \ln\left\{\frac{p(1-r-a+rp)}{(1-p)(a-rp)}\right\} = \frac{\Delta}{kT} \equiv f_2(\phi)$$

Calculations were done in a numerical manner with the C++ language.

3. Results

Figure 1 shows the calculational result of the Bragg-Williams model with atom A and B, for the composition of A atom $a = r = 1/2$, and the interaction coefficient J as 20.83 meV, and the coordination number z as 6, 8, 12, respectively. The equilibrium order parameters are obtained by solving the equation $f_1(\phi) = f_2(\phi)$ in a self-consistent way at each value of the temperature T. We obtained the interaction coefficient J from the case of Fe3Al, which is FCC structure and has the order-disorder critical temperature, at which complete disorder becomes unstable, as 1450 K. The results clearly show the decreasing behavior of the order parameter of the system with respect to the increase of the temperature, and the critical temperatures are obtained from the relations between the Bragg-Williams model and the Bethe model:

$$\Delta_0 = 2r(1-r)^{-2}(q-a)zJ$$

where Δ_0 is the increasing energy caused by the one position of disorder. Then the critical temperature of the system would be

$$T_c = (2zJ/k)a(1-a)r(1-r)^{-1}.$$

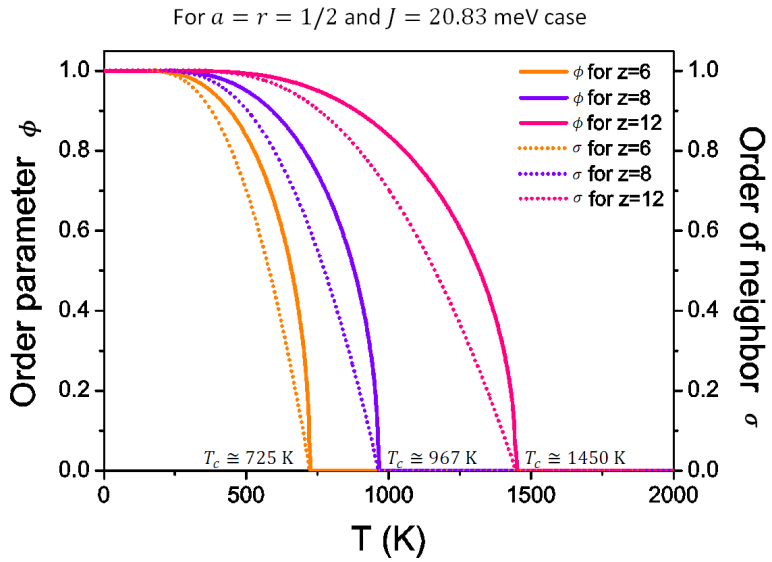

Fig. 1 Calculated results of the Bragg-Williams model with interaction coefficient J = 20.83 meV, and the coordination number z = 6, 8, 12, respectively. The order parameter decreases as the temperature increases, until it becomes zero at the critical temperature.

4. References

[1] W. L. Bragg and E. J. Williams, Proc. R. Soc. Lond. A **145**, 699-730 (1934).

[2] W. L. Bragg and E. J. Williams, Proc. R. Soc. Lond. A **151**, 540-566 (1935).

[3] W. L. Bragg and E. J. Williams, Proc. R. Soc. Lond. A **152**, 231-252 (1935).

[4] H. A. Bethe, Proc. R. Soc. Lond. A **150**, 552-575 (1935).

[5] G. Inden. Acta. Metall. **22**, 945-951 (1974).