Calculation of Thermodynamic Properties of κ-carbide by Wang-Landau Algorithm

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1. Introduction

Due to the increasing needs of high strength light weight steels, the importance of $(Fe, Mn)_3AlC$ κ-carbide is getting higher. Uniformly distributed nano-size κ-carbides in an austenite matrix supports a shear-band plasticity (SIP effect), and highly improves the strength and ductility of Fe-Mn-Al-C light-weight steel, so results in excellent mechanical properties[1]. In this work, we set the cell gas model of Fe_2MnAlC, and with this model we calculated its thermodynamic properties by Wang-Landau Monte Carlo simulation.

2. Calculation method

We calculated formation enthalpy of Fe_2MnAlC for six states based on the magnetism and the carbon occupation at octahedra[2]. The First-Principles calculations were done by all-electron full potential linearized augmented plane-wave method(FLAPW)[3]. After that, the cell gas model of Fe_2MnAlC was set from these values. The 'cell gas' means, a bulk of solid that is made up of several unit cells, and these cells act like gas, i.e., without interaction. Our model is similar to the 3D ising model, and consists of L×L×L cells that may have 6 different states. So these L×L×L cells make up a bulk of Fe_2MnAlC.

With this model, the partition function calculation of Fe_2MnAlC was done by the Wang-Landau algorithm[4], which is one of the Monte Carlo simulation method. If a random walk is performed in energy space with a probability proportional to the reciprocal of the density of states $g^{-1}(E)$, then a flat histogram is generated for the energy distribution. At first, densities of states of all energy space are set for 1. Then the random walk begins in energy space by flipping state randomly. If E_1 and E_2 are energies before and after a state is flipped, the transition probability from E1 to E_2 is

$$p(E_1 \rightarrow E_2) = \min\left[\frac{g(E_2)}{g(E_1)}, 1\right] \tag{1}$$

Each time an energy level E is visited, the corresponding g(E) is updated by a modification factor f, i.e. g(E)f. This process is done iteratively until the histogram H(E) is "flat", and then f is reduced to $\sqrt{f}$. We kept doing this until $f=\exp(10^{-8})$. From the final densities of states, the partition function over whole energy space was made. The classic partition function can be written as a sum over all energies, so

$$Z = \sum_i e^{-E_i/k_B T} \equiv \sum_E g(E) e^{-E/k_B T}$$

where g(E)s over energy space are the densities of states. And these g(E)s are independent of the temperature, so they can be used to find properties of the system at any temperatures. From the partition function Z, thermodynamic properties can be derived: the Helmholtz free energy $F(T) = -k_B T(\ln Z)$, the internal energy $U(T) = \langle E \rangle_T \equiv \Sigma_E E g(E) e^{-\beta E}$, the entropy $S(T) = [U(T) - F(T)]/k_B T$, and the specific heat $C(T) = [\langle E^2 \rangle_T - \langle E \rangle_T^2]/k_B T^2$.

3. Results

Fig. 1 shows the result of calculation for L=3. All values were divided by N = L×L×L. (b) and (d) have large fluctuations, and it is thought that these fluctuations came from the size effect.

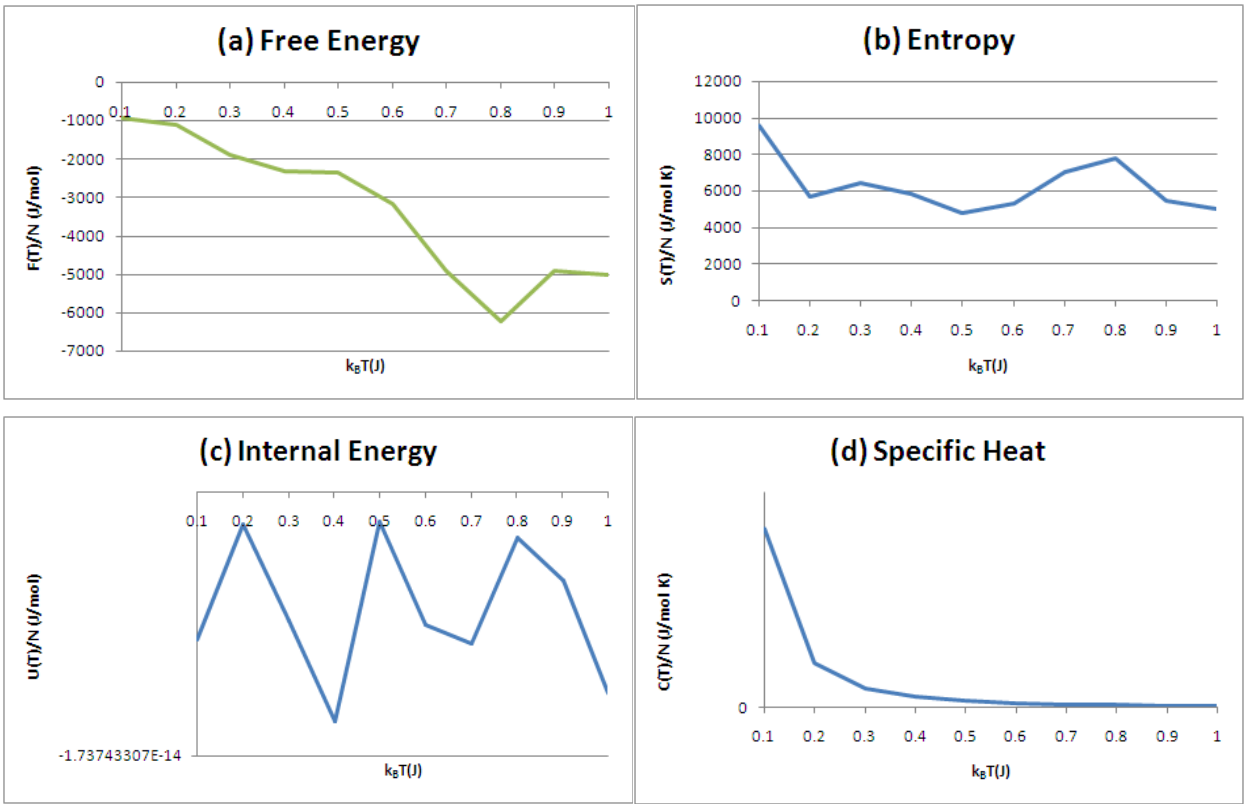

Fig. 1. Calculated results of L=3 case. (a) Free energy (b) Internal energy (c) Entropy (d) Specific heat. The *x* axis of each graph is k_BT(J), and the y axis is the value of each thermodynamic property (J/mol or J/mol K).

4. References

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