Wang-Landau Monte Carlo calculation for thermodynamic properties of κ-carbide

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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 Fe2MnAlC, and with this model we calculated its thermodynamic properties by Wang-Landau Monte Carlo simulation.

2. Calculation method

We calculated the 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]. The cell gas model of Fe_2MnAlC was built from these values. The 'cell gas' means, a bulk solid 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.

The partition function calculation of Fe_2MnAlC was done by the Wang-Landau Monte Carlo method [4]. 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. 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 probability of transition from E_1 to E_2 is

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

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 $\sqrt{f}$. And from the final densities of states, the partition function over whole energy space was made. The classical partition function can be written as a sum over all energies, so

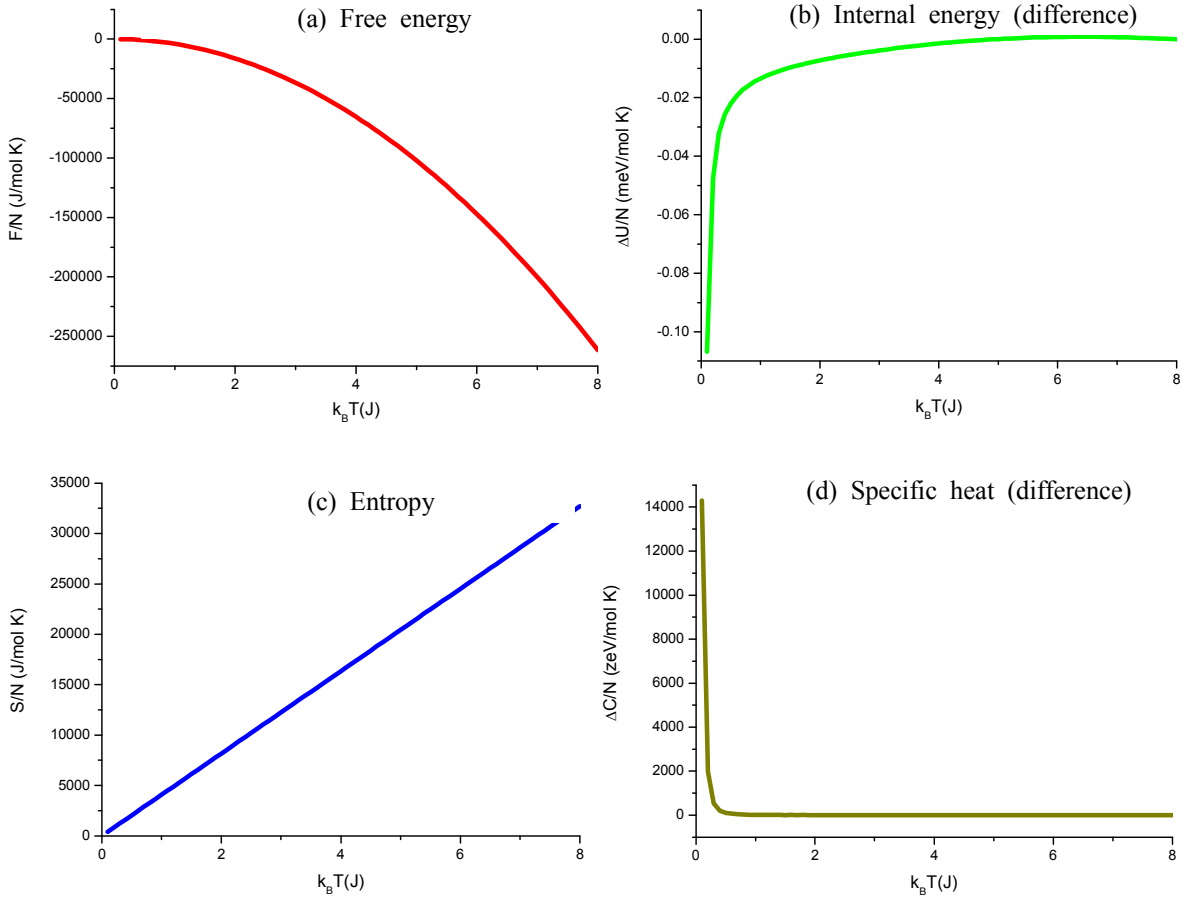
$$Z = \sum_i e^{-E_i/k_B T} \equiv \sum_E g(E) e^{-E/k_B T}$$

and from the partition function Z, thermodynamic properties of κ-carbide was be derived.

3. Results

Fig. 1 shows the result of calculation for L=10. All values were divided by N = L×L×L.

Fig. 1. Calculated results of L=10 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.



The interaction between each cell is not considered in our model, so the free energy almost simply decreases as temperature increases. But at very low temperature, the gradient of free energy curve changes. This behavior seems as the critical phenomenon of the system, i.e., the phase transition, and it happens near 0 K. We didn't yet evaluate the detailed behavior of the system in the vicinity of critical temperature.

The internal energy is almost constant, but as in the free energy case, it shows the critical phenomenon near 0 K. The specific heat also shows the critical phenomenon, an is almost zero at higher temperature. This is explained by $C = \partial U / \partial T$, and the fact that U stays almost constant over the critical temperature.

4. References

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