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Calculating Heat Capacities of FCC Metals via Monte-Carlo Method

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Abstract

The metals of Aluminum (Al), Copper (Cu) and Nickel (Ni) are used in a wide range of industries. Aluminum, for example is used in airplanes and many other transportation vehicles. Copper is used in wires, and Nickel is used in making gas turbines. All of these three metals have a face-centered cubic (FCC) structure, in which atoms are located at each corner of a cubic unit cell and at the center of all cubic faces. In this paper, the heat capacities of Al, Cu and Ni are studied via Monte Carlo method.

Keywords: Aluminum; Copper; Nickel

Introduction

A total of 256 atoms with 4 × 4 × 4 cubic unit cells are considered in this paper. The Morse potential is used to model the interatomic interaction between two atoms having a distance of r:

$$W(r) = D_e\left[e^{-2\beta(r-r_0)} - 2e^{-\beta(r-r_0)}\right] \quad (1)$$

Where the Morse potential parameters [1,2] for different materials are listed in Table 1.

The Monte Carlo method is used here to calculate the average energy per atom at different temperatures in the simulated molecular model. Then, the heat capacity can be evaluated via the following equation:

$$C_v = \frac{\Delta E_{avg}}{\Delta T.M} \quad (2)$$

Where, ΔE_{avg} is the difference of averaged energy per atom and ΔT is the temperature difference. M is the atomic mass which is 4.48039E-23 g/atom for Al, 1.05444E-22 g/atom for Cu and 9.74627 g/atom for Ni respectively.

It should be noted that the volume of the simulated model was kept the same during the Monte Carlo simulation. The averaged energy per atom was calculated at various temperatures between 200 K and 290 K. The simulation procedure of the Monte Carlo method i.e., the Metropolis method is briefly summarized as below:

(1) Input variables: The number of atoms, the temperature and the Morse potential parameters are given.

(2) Initialization: Based on the input variables, the positions of the atoms are identified, and the initial energy is calculated.

(3) Iteration: The maximum number of iterations is given so that the model will reach to the equilibrium state eventually at a given temperature.

(3-1) Trial movement: One atom is randomly selected and then given a small displacement perturbation.

(3-2) Energy evaluation: The energy change, ΔE after the trial movement is calculated.

Material	D_e(ev)	r_0(A)	β(A^{-1})	Lattice constant (A)
Al	0.2703	3.253	1.165	4.05
Cu	0.3429	2.866	2.359	3.62
Ni	0.4205	2.780	1.4199	3.52

Table 1: Morse potential parameters for Al, Cu and Ni.

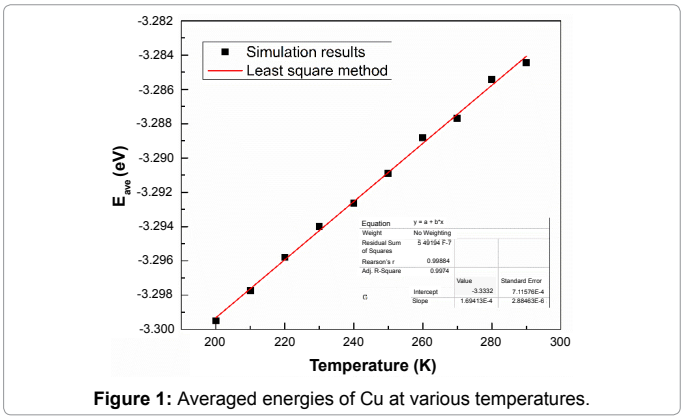

Figure 1: Averaged energies of Cu at various temperatures.

(3-3) If the energy change is negative, the trial movement will be accepted, and the next iteration will be processed.

(3-4) If the energy change is positive, a random number will be generated. If this random number is smaller than $e^{-\Delta E/Kt}$

Where, k is the Boltzmann constant, the trial movement will be accepted. Then, the next iteration will be processed.

(4) Calculation of the averaged energy per atom.

Figure 1 shows the averaged energies of Cu at various temperatures based on Monte-Carlo simulations. A linear function is used to fit the simulation results so that the slope can be used to calculate the heat capacity. The calculated heat capacities of three metals are listed in Table 2 and compared to the reference ones [3].

Conclusion

It can be seen that the calculated heat capacities are lower than the reference ones. It is due to the Morse potential function we used in this paper. The Morse potential is a simple one which only describes

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Material	Heat capacity *J/(gK)*	Reference [3]
Al	0.744	0.910
Cu	0.254	0.385
Ni	0.205	0.444

Table 2: Heat capacities of Al, Cu and Ni.

the interaction between two atoms. The potential due to bond angle bending and torsion usually play an important role on mechanical properties of crystalline solids. For metals, the widely used potential function is the embedded atom method (EAM) [4].

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