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Critical temperature of the Ising ferromagnet on the fcc, hcp, and dhcp lattices

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HIGHLIGHTS

- First Ising critical temperatures calculated on the hcp and double hcp lattices.
- Ising critical temperature on the fcc lattice with unprecedented precision.
- The hcp lattice has higher critical temperature than the fcc and double hcp lattices.

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ABSTRACT

By an extensive Monte-Carlo calculation together with the finite-size-scaling and the multiple histogram method, the critical coupling constant ($K_c = J/k_B T_c$) of the Ising ferromagnet on the fcc, hcp, and double hcp (dhcp) lattices were obtained with unprecedented precision: $K_c^{\mathrm{fcc}} = 0.1020707(2)$, $K_c^{\mathrm{hcp}} = 0.1020702(1)$, and $K_c^{\mathrm{dhcp}} = 0.1020706(2)$. The critical temperature T_c of the hcp lattice is found to be higher than those of the fcc and the dhcp lattice. The dhcp lattice seems to have higher T_c than the fcc lattice, but the difference is within error bars.

1. Introduction

The Ising model is an important model in condensed matter physics and statistical mechanics [1]. Although it is simple, it can be solved analytically only in one and two dimensional systems [2–4]. In three dimensional cases we should resort to numerical methods. There have been many works for the simple cubic lattice, but other lattices have not been studied enough. Especially, results on the close-packed lattices such as the face-centered-cubic (fcc), the hexagonal close-packed (hcp), and the double hexagonal close-packed (dhcp) lattices are rare, though they are important lattice structures.

In this work, we studied the ferromagnetic Ising model on the three close-packed lattices (fcc, hcp, and dhcp) to compare their critical temperatures. They share many properties. All of them are close-packed structures with the same dimensionality, packing ratio, and coordination number. They are different only in the stacking sequence. (See Fig. 1 for more details.) Therefore, we expect they have similar transition temperatures. However, it is not trivial to conclude whether they have exactly the same critical temperature. In the case of percolation threshold, it was shown that fcc and hcp lattices have the same bond percolation threshold within error bars, but different site percolation thresholds [5]. By extensive Monte-Carlo calculations with the multiple histogram method [6] and the finite size scaling [7], we conclude that the hcp lattice has higher critical temperature T_c than the fcc and the dhcp lattice. The dhcp lattice seems to have higher T_c than the fcc lattice, but the difference is within error bars.

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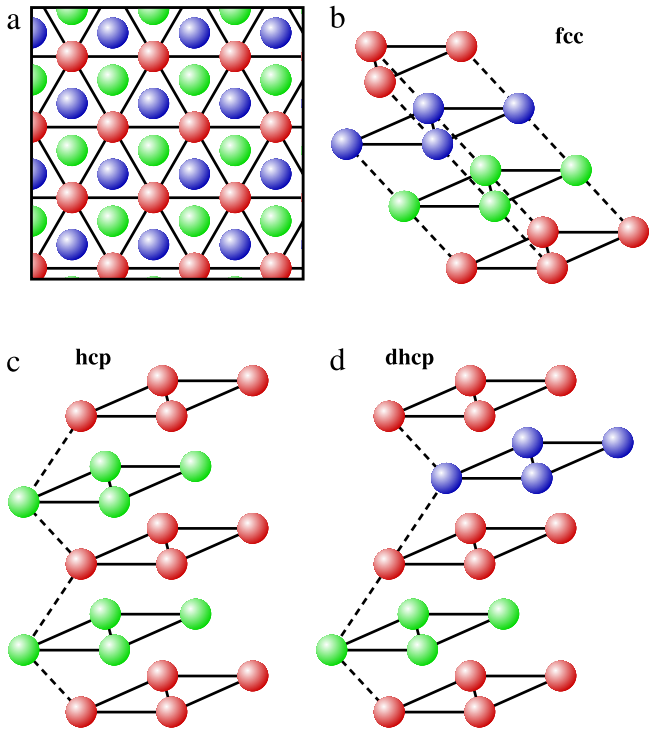

Fig. 1. The lattice points of fcc, hcp, and dhcp structures. (a) shows the lattice points projected on the *xy*-plane for A (red), B (green), and C (blue) layers. In the fcc lattice, layers are stacked by A–B–C–A–B–C–· · ·. In the hcp and dhcp lattices, the stacking sequences are A–B–A–B–· · · and A–B–A–C–A–B–A–C–· · ·, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2. Model and method

The Ising model Hamiltonian studied in this work is as follows.

$$H = -\sum_{\langle i,j\rangle} J S_i S_j. \tag{1}$$

The spin at the ith site S_i may take the values of $+1$ or -1, only. The summation runs for all the nearest neighbor pairs, excluding double counting. The coupling constant J is assumed to be positive (ferromagnetic interaction). It is customary to define the dimensionless coupling constant $K = J/k_BT$ and the dimensionless energy $E = -\sum_{\langle i,j\rangle} S_iS_j$.

The calculation was done for parallelepiped clusters of size $L \times L \times L$ with the periodic boundary condition. Ten values of L were chosen from $L = 32$ to $L = 256$. Since the lattice size is large, the exact enumeration is impossible and we used the Monte-Carlo method. To investigate near the critical temperature, we used the Wolff single-cluster algorithm [8], which is free from the critical slowing down. It is more efficient than the Swendsen–Wang algorithm [9], especially in three dimensional lattices [10]. We confirmed that the three algorithms (Metropolis, Wolff, and Swendsen–Wang) give consistent and equivalent results.

To obtain precise information near the critical temperature, we used the multiple histogram method [6], which is an extension of the single histogram method [11]. The histogram $h_0(E)$ and average of a quantity $\langle X\rangle^E_{K_0}$ as a function of energy are calculated at a given coupling K_0 by the Monte-Carlo importance sampling [$h_0(E) \propto \exp(-K_0E)$]. They are used to find the thermodynamic average of the quantity X at another coupling K by reweighting:

$$\langle X\rangle_K = \frac{\sum_E \langle X\rangle^E_{K_0}\ h_0(E)\ \mathrm{e}^{(K_0-K)E}}{\sum_E h_0(E)\ \mathrm{e}^{(K_0-K)E}}. \tag{2}$$

Since this method uses the overlap of the two histograms at different coupling constant, the error increases as $|\langle E\rangle_K - \langle E\rangle_{K_0}| \approx cN|1/K_0 - 1/K|$, where $N = L^3$ is the number of sites and $c = [\mathrm{d}\langle E\rangle_K/\mathrm{d}(1/K)]/N$ is the specific heat. If the number of Monte-Carlo steps is large enough, we can obtain the thermodynamic information over wide range around the coupling constant K_0. However, it becomes more and more difficult as the lattice size increases. Rather than to simulate more at a single coupling constant, it is more efficient to simulate multiple times at different coupling constants K_i to get reliable