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Exchange interaction and magnetic phase transition in layered Fe/Au superlattices

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Abstract

In order to study the finite-temperature properties of the layered Fe/Au superlattice, Monte Carlo (MC) simulations are carried out based on a Heisenberg model with the exchange parameters extracted from the ab initio total energies and a phenomenological anisotropy constant. It is argued that the Curie temperature is rather insensitive to the anisotropy and is essentially determined by the ab initio exchange parameters. Due to the reduced coordination number of the magnetic atoms at interfaces, the Curie temperature obtained by this ab initio-MC scheme decreases as decreasing of Fe layer thickness is governed essentially by Weiss'law. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Exchange interaction; Curie temperature; Ferromagnetic multilayer; Monte Carlo simulation

Fe/Au systems have received much attention both experimentally [1,2] and theoretically [3–5]. Although the theoretical works have given good understanding to the ground-state magnetism, the finite-temperature magnetism, which is more important for practical use, is still a challenging problem to theoretical research. Recently, Rosengaad and Johansson [6] examined the finite-temperature properties of ferromagnetic BCC Fe, FCC Co and Ni by using the Monte Carlo (MC) simulation with the exchange parameters deduced from the linear-muffin-tin orbital atomic-sphere approximation total energy of selected spiral spin-density wave magnetic structures. Zhou et al. [7] used a similar procedure to study the magnetic phase transitions in FCC Fe and Mn antiferromagnets with exchange parameters obtained by fitting to total energy of frozen collinear magnetic states.

In the present study, we apply the ab initio-MC method on the layered Fe/Au superlattice. First we extract the exchange parameters from the obtained ab initio total energies using the self-consistent full-potential linearized augmented-plane-wave (FLAPW) method. Then, based on the Heisenberg model, we use the exchange parameters to perform MC simulations to study the finite-temperature magnetic properties.

In Fig. 1, the values of the direct exchange energy, $J_L(d)$ as a function of the Fe interlayer distance d, are presented for $Fe_n/Au(0\,0\,1)$ ($n = 5, 7, 9$) systems. It is shown that (1) interlayer exchange interaction exhibits similar behavior in the three different systems, indicating that the exchange interaction can be regarded as a unique function of the distance in the thick layered Fe systems; (2) the exchange interaction is relatively short ranged, the dependence of the coupling strength on the distance shows a weak oscillatory behavior, and at large distance, it approaches to zero quickly; (3) the NN interlayer exchange coupling is strongly ferromagnetic (~ 17.5 mRy), while the NNN interlayer exchange coupling is weak antiferromagnetic (~ -2.3 mRy). These facts indicate that in the layered BCC-Fe/Au superlattices the dominating exchange interactions are ferromagnetic.

Using the exchange parameters deduced from the FLAPW total energy of selected magnetic structures, classical MC simulations with the standard Metropolis algorithm are carried out with system sizes $s \times s \times n \sim 5000$, and ~ 6000 MC steps. Three-dimensional (3D) periodic boundary are adopted for BCC Fe and two-dimensional (2D) periodic boundary conditions with free interface boundary conditions are adopted for

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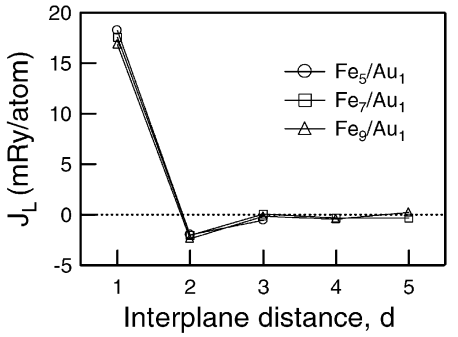

Fig. 1. Interlayer exchange parameter, J_L, as a function of the distance d ($d = |i - j|$) between the i and jth Fe planes in the BCC-Fe/Au multilayers.

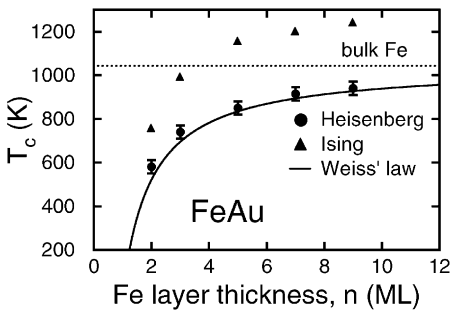

Fig. 2. Dependence of the Curie temperature on the Fe layer thickness (n). Solid circles indicate the Heisenberg–MC results, triangles indicate the Ising–MC ones. Solid line represent the Weiss' law expressed by $T_c(n) = T_c^{bulk}(1 - 1/n)$.

$Fe_n/Au(0\,0\,1)$ systems with $n = 2$, 3, 5, 7 and 9. T_c for BCC Fe is estimated to be 1057 K, which is fairly in good agreement with 1043 K of experimental value and is very close to theoretical results 1060 K given by Rosengaad and Johansson [6]. In Fig. 2, T_c as the functions of Fe layer thickness n are shown. It is seen that T_c is a smooth increasing function of Fe layer thickness, which increases from 582 to 1057 K as the Fe layer thickness increases from 2 ML to bulk. T_c estimated from the Weiss' law and obtained from the Ising model are also plotted in Fig. 2. It is shown that while the general behavior is essentially governed by Weiss' law, there are remarkable discrepancies between the calculated results and the Weiss' law result, especially for thinner systems. The physics accounting for such discrepancy is the enhanced exchange energy in thinner systems due to the interface effect [3]. On the other hand, T_c obtained from the Ising model are much larger than those from Heisenberg model always and certainly even larger than experiments. This fact indicates that the neglecting of the variational freedoms of spin leads to small fluctuation probability and higher transition temperature.

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