Exchange interaction and magnetic phase transition in layered Fe/Au(001) superlattices

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Ab initio calculations for layered Fe/Au(001) superlattices with a set of collinear spin configurations are performed by means of the self-consistent full-potential linearized augmented-plane-wave method under the generalized gradient approximation. To study the finite-temperature magnetism of such superlattices, 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 governed essentially by Weiss' law. These results are discussed in connection with recent experimental and theoretical studies.

I. INTRODUCTION

Recent technical progress now makes it possible to synthesize high quality artificial ultrathin films with stable or metastable lattice geometries in layer by layer growth mode. Because of the existence of interface or surface states and the different environment relative to bulk in the layered magnetic systems, novel physical properties such as the enhanced magnetoresistance, large magnetic moment, and perpendicular magnetic anisotropy are induced.[1] One such system, the Fe/Au multilayer, has received much attention both experimentally[2–9] and theoretically.[10–16] Although neither intermediate phase nor intermetallic compound exists naturally in the equilibrium phase diagram, experimentally, the metastable $L1_0$ FeAu alloys[2] and layered bcc Fe/Au(001) multilayers[2,3] can be fabricated artificially by the molecular beam epitaxy technique. It has been reported that the $L1_0$ FeAu ordered superlattice is ferromagnetic with enhanced magnetic moment and perpendicular anisotropy,[2] and fine layered Fe/Au multilayers show novel magneto-optical Kerr spectra.[3] These special properties make them very interesting for applications to sensors, communication devices, or recording media and so on.[1]

Several theoretical studies including ours have been performed on the magnetic and electronic properties of FeAu systems.[10–16] These theoretical works have revealed the ground state behaviors such as the stabilities of spin configurations,[14] the interplay between magnetization and equilibrium volume,[14,15] the magnetic anisotropy,[16] and so on. From these theoretical studies, the stable magnetic structures, especially some antiferromagnetic configurations can now be predicted by comparing total energies; and equilibrium atomic geometry as well as lattice constants can also be determined. However, although these theoretical works have given good understandings to the ground state magnetism, the finite-temperature magnetism, which is more important for practical usage, is still a challenging problem to theoretical researchers.

On the finite-temperature magnetism, several pioneering theoretical works have been successfully performed on the bulk magnetic metals. You *et al.*[17] calculated exchange parameters of bcc Fe from the selected four types of spin arrangements, and estimated the Curie temperature by the mean-field theory. Based on an idea of disordered alloy analogy, Oguchi *et al.*,[18] Pindor *et al.*,[19] and Gyorffy *et al.*[20] made a direct calculation of the electronic structures at finite temperature of the transition metals with the local spin-density approximation (LSDA), using the coherent potential approximation to realize the paramagnetic state. Moreover, Liechtenstein *et al.*[21] suggested a convenient form of the exchange constants constituted of quantities obtained at the ground states from the LSDA calculations, and used it on Fe, Ni, and Ni-Pd alloys. Luchini and Heine[22] studied the short-range order around the Curie temperature and revealed that to a first approximation Fe behaves as a Heisenberg ferromagnet. Staunton and Gyorffy[23] calculated the paramagnetic susceptibilities and the Curie temperatures of bcc Fe and fcc Ni within a first-principles framework for Onsager cavity field. Uhl and Kübler[24] investigated the finite-temperature properties of Fe, Co, and Ni by employing an exchange-

coupled spin-fluctuation theory. Recently, Rosengaad and Johansson[25] examined the finite-temperature properties of ferromagnetic bcc Fe, fcc Co, and Ni by using the Monte Carlo (MC) simulations 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.*[26] used a similar procedure to study the magnetic phase transitions in fcc Fe and Mn antiferromagnets but with exchange parameters obtained by fitting to the total energies of frozen collinear magnetic states. The method proposed by the last two groups, namely the *ab initio* MC method, most approaches to the first principles at present stage to our knowledge, so that the Curie temperatures determined by this method are the best estimations compared with experiments up to now.[25,26]

In the present study, with the layered Fe/Au(001) system as an example, we show that the method can be extended to study the low-dimensional systems. The organization of the present paper is as follows. First, the total energies of the possible collinear spin configurations are calculated by means of the self-consistent full-potential linearized augmented-plane-wave (FLAPW) method, and the exchange parameters are extracted from *ab initio* results within a classical Heisenberg model. Then, two examples, the bulk bcc Fe and Fe_2/Au_2 superlattice are given to show how the method works. Finally, the comparisons with the experiments are made, and the general trends for T_c versus Fe layer thickness are analyzed.

II. EXCHANGE INTERACTIONS IN LAYERED FE/AU(001) SUPERLATTICES

All the calculations reported in the present paper are performed by using the self-consistent FLAPW (Ref. 27) method under the generalized gradient approximation (GGA) (Ref. 28) in a scalar relativistic version without spin-orbit coupling (SOC). The bcc-Fe/Au(001) superlattices consisting of Fe (001) and Au (001) monolayers (ML) are considered as fcc-like superlattices.[13] The in-plane lattice parameter a is set to 4.08 Å, which is consistent with fcc Au lattice constant. The layer spacing of Fe-Fe, and Au-Au are set to 1.44 and 2.04 Å in corresponding to the bulk values of bcc Fe and fcc Au, respectively, and the layer spacing of Fe-Au is fixed to 1.76 Å as a close-packed atom arrangement (no interlayer spacing relaxations). The radii of the muffin-tin spheres are set to 1.44 Å for Au and 1.24 Å for Fe, respectively. The Brillouin zone sampling is performed using 36–156 special k points in the irreducible Brillouin zone. Convergence of the total energy and the charge is carefully checked throughout this calculation.

In order to study the exchange interactions in the layered Fe/Au superlattices, we have calculated the total energies of all the possible collinear spin configurations allowed by the inversion symmetry [including $c(2\times2)$ in-plane antiferromagnetic] within the fcc-like superlattices (see Ref. 13 for the supercell structure). In Table I, we select some spin configurations to show their total energies (E_T) and magnetic moments (M). Each spin configuration calculated can be regarded as a special case of the helical structure. The obtained *ab initio* total energies for arbitrary magnetic structures can be simply expressed by the following classical Heisenberg model:

$$E_T = E_{\mathrm{PM}} - \sum_i E_M - \frac{1}{2}\sum_{i,j} J_{r(ij)}\vec{\sigma}_i\vec{\sigma}_j, \tag{1}$$

where E_{PM} is the total energy in the paramagnetic (PM) state, E_M the single-ion magnetizing energy coming from the spin-polarization on magnetic site, $\vec{\sigma}_i$ is a unit vector representing the spin direction of the ith site, $J_{r(ij)}$ are the exchange integrals, and the summation runs over all pairs of the corresponding magnetic atoms on ith and jth sites. The exchange coupling $J_{r(ij)}$ as a function of the distance $r(ij)$ must be a long ranged set in principle, and the long ranged interaction might be important for those highly frustrated systems such as fcc Fe and fcc Mn.[26] However, for bcc Fe-based systems the exchange interaction is found to be relatively short ranged (see, for example, Ref. 25), the main contribution to the exchange energy comes from the interaction up to third nearest neighbors (see Table II), so that the first several terms are usually believed to be enough to capture the main physics.

Let us first study the *interlayer* exchange coupling $J_L(d)$ as a function of the Fe interlayer distance d, which can be easily related with the interatomic exchange parameters J_r defined in Eq. (1). For example, the nearest neighbor (NN) interlayer exchange coupling $J_L(1)=4J_1+8J_4+\cdots$, and the next nearest neighbor (NNN) interlayer $J_L(2)=J_2+4J_3+4J_5+\cdots$, and so on, where J_1, J_2, J_3 are the interatomic exchange parameters with index (1, 2, 3, etc.) labeling the distances. By least square fitting technique, $J_L(d)$ as a function of d are obtained and plotted in Fig. 1 for $Fe_n/Au(001)$ ($n=5$, 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 ($\sim$17.5 mRy), while the NNN interlayer exchange coupling is weak antiferromagnetic (~ -2.3 mRy). These facts indicate that in the layered bcc-Fe/Au superlattices the dominating exchange interactions are ferromagnetic [the most stable magnetic configurations are ferromagnetic, in contrast, the most unstable magnetic configurations of layer-by-layer antiferromagnetic ($+-+-+-$) with nearest neighbor interlayer antiferromagnetic coupling as shown in Table I], so that the spin arrangement within Fe film should be ferromagnetic.

On the contrary, quite different properties have been reported by Asada *et al.*,[29] Zhou *et al.*,[30] and Szunyogh *et al.*[31] for fcc-Fe/Cu system, where the frustration exists. Strong antiferromagnetic couplings between the NNN layers are found for both the interface and interior layers in fcc-Fe/Cu system, which are responsible for the bilayer antiferromagnetic ground state configuration.[30] For fcc-Fe_n/Ag(100) [Fe free surface on Ag(100), $n\leqslant 16$], Sommers *et al.*[32] found that the most stable magnetic configurations are ferromagnetic. These results suggest that the magnetic behaviors of Fe-

TABLE I. Spin configuration, total energy E_T (relative to paramagnetic states) in mRy per unit cell, and sum moments M (μ_B) for ideal bcc-Fe/Au(001) superlattices. Plus and minus shown in the first column represent the spin directions in Fe layers. Data starting from the fourth column are moments of each Fe layer from interface (I) through the inner layer.

System	E_T (mRy)	M (μ_B)	Fe_I	Fe_{I-1}	Fe_{I-2}	Fe_{I-3}	Fe_{I-4}
Fe_9/Au_1							
+ − + − + − + − +	−101.7	2.626	2.233	−1.970	1.945	−1.887	1.920
+ + − + − + − + +	−179.5	7.488	2.601	2.067	−1.902	1.948	−1.952
+ − + − − − + − +	−184.8	2.284	2.349	−2.065	1.901	−2.131	−2.500
+ − + + − + + − +	−193.6	6.667	2.273	−2.031	2.115	2.073	−2.211
+ − − + − + − − +	−196.9	1.972	2.349	−2.297	−2.134	2.021	−1.899
+ − + + + + + − +	−248.1	12.496	2.387	−1.929	2.160	2.449	2.469
+ + − + + + − + +	−253.0	12.437	2.659	2.138	−1.974	2.209	2.446
+ + + − + − + + +	−256.5	13.186	2.729	2.489	2.211	−1.814	2.041
+ − − − + − − − +	−261.8	7.035	2.305	−2.265	−2.494	−2.161	2.029
+ + − − + − − + +	−267.4	2.473	2.572	2.157	−2.302	−2.193	1.968
+ − − + + + − − +	−275.4	1.990	2.294	−2.348	−2.301	2.164	2.423
+ − − − − − − − +	−300.3	11.317	2.154	−2.171	−2.325	−2.264	−2.269
+ + + + − + + + +	−316.8	17.179	2.710	2.488	2.464	2.081	−2.121
+ + − − − − − + +	−329.8	1.644	2.658	2.213	−2.195	−2.381	−2.386
+ + + − − − + + +	−338.2	8.121	2.707	2.446	2.258	−2.110	−2.482
+ + + + + + + + +	−375.8	21.728	2.719	2.424	2.386	2.320	2.307
Fe_7/Au_1							
+ − + − + − +	−87.7	2.616	2.210	−1.976	1.975	−1.865	
+ − + + + − +	−171.4	7.843	2.359	−1.915	2.231	2.496	
+ + − + − + +	−176.0	7.633	2.657	2.100	−1.913	1.960	
+ − − + − − +	−183.2	1.950	2.365	−2.318	−2.140	2.180	
+ + + − + + +	−240.8	12.720	2.702	2.477	2.206	−1.969	
+ − − − − − +	−244.8	6.991	2.305	−2.224	−2.455	−2.452	
+ + − − − + +	−246.3	2.918	2.654	2.203	−2.212	−2.435	
+ + + + + + +	−301.9	17.054	2.687	2.369	2.390	2.288	
Fe_5/Au_1							
+ − + − +	−77.1	2.951	2.450	−1.870	1.769		
+ + − + +	−149.4	7.476	2.689	2.125	−2.132		
+ − − − +	−158.0	2.191	2.363	−2.240	−2.510		
+ + + + +	−214.2	12.743	2.729	2.454	2.487		
Fe_4/Au_2							
+ − − +	−115.57	0.143	2.389	−2.331			
+ + + +	−172.22	10.443	2.729	2.526			
Fe_3/Au_1							
+ − +	−59.2	3.010	2.476	−2.011			
+ + +	−133.6	7.860	2.713	2.464			
Fe_2/Au_2							
+ +	−180.8	11.184	2.765	2.765			

based superlattice are very sensitive to the detailed atom distributions and coupling distances.[33]

In Table II, the exchange parameters (J_1, J_2, J_3) between the first three neighbors and E_M are listed. These parameters will be used in the MC simulations to study the finite-temperature properties as shown in the next chapter. For each system reported, the fitting error of the total energy variation is about 2.7−3.4%. Thus the underlying interactions have been accounted for mostly. Since the longe ranged set of the exchange parameters have been truncated, every single parameter does not possess a *clear* physical meaning. However, it is interesting to define a quantity $J_{\text{eff}} = \Sigma_{i,j} J_{r(ij)}/(8N) \simeq (8J_1 + 6J_2 + 12J_3)/8$, which has the physical interpretation of the effective exchange coupling renormalized to the NN pair (see Table II). This quantity is rather insensitive to how many parameters retained in the fitting procedure. We find that this effective exchange parameter J_{eff} increases as the Fe layer thickness decreases, clearly demonstrating that the interface enhances the exchange interaction. Following Refs. 30,31, in order to study the surface effect more explicitly, we also separately determined the exchange interaction related to the surface layers

TABLE II. Magnetization energy (E_M), exchange integrals (J_1, J_2, J_3) and *effective* exchange coupling J_{eff} [$=(8J_1+6J_2+12J_3)/8$] renormalized on the NN pair for FeAu superlattices.

System	E_M (mRy)	J_1 (mRy)	J_2 (mRy)	J_3 (mRy)	J_{eff} (mRy)
Fe_2/Au_2	35.0	4.122	1.378	−0.398	4.56
Fe_3/Au_1	32.5	4.806	0.696	−0.706	4.47
Fe_5/Au_1	29.8	4.285	0.991	−0.748	3.91
Fe_7/Au_1	28.8	4.391	1.021	−0.874	3.85
Fe_9/Au_1	27.9	4.271	1.510	−1.077	3.79
bcc Fe	25.1	4.209	1.648	−1.057	3.86

(J_0) and that related to the inner layers in the least square fitting procedure. On the contrast to fcc-Fe/Cu multilayers where the inhomogeneity of exchange coupling may play an important role,[30] we find that there is typically only 5% enhancement in J_0 compared with J_1 of NN inner layers. Actually, such an enhancement effect have been implicitly included in our present definition of $J_{r(ij)}$. The increase of J_{eff} in Fe_2/Au_2 reaches 20% compared to bulk Fe. Moreover, E_M, indicating the on-site magnetization energy, is also a decreasing function of Fe layer thickness due to the enhanced magnetic moments.[13]

III. MONTE CARLO SIMULATION OF PHASE TRANSITION

Using the effective exchange parameters given in Table II, classical MC simulations 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 periodic boundary conditions with free interface boundary conditions are adopted for $Fe_n/Au(001)$ systems with $n=2,\ 3,\ 5,\ 7$, and 9.[34] For each system, the magnetization M, the specific heat $C=[\langle E^2\rangle-\langle E\rangle^2]/k_BT^2$, and the susceptibility $\chi=[\langle M^2\rangle-\langle M\rangle^2]/k_BT$ are obtained as a function of the temperature, where k_B is Boltzmann's constant. In principle, Curie temperature T_c can be estimated from the peak of the specific heat or from the magnetic susceptibility according to Curie-Weiss' law. While the actual values of the specific heat and magnetic susceptibility depend on the system size, in order to accurately determine the transition temperature T_c, the fourth-order cumulant $U_L=1-\langle M^4\rangle_L/3\langle M^2\rangle_L^2$ is also calculated. Theoretically, for $T<T_c$, U_L tends to 2/3, and for $T>T_c$, U_L decreases toward zero.[35] This behavior of the cumulant makes it very useful to estimate of T_c, which is not biased by any assumption about the critical exponents. In the present study for each system, U_L versus temperature for various system sizes are plotted and T_c are estimated from the common intersection point of the U_L curves.[35]

In Fig. 2, the magnetization (M), the fourth-order cumulant (U_L), and the specific heat (C) for bcc Fe are shown as the functions of temperature, respectively. From the calculated U_L-T curve, T_c for bcc Fe is estimated to be 1057 K, which is in fairly good agreement with 1043 K of experimental value[36] and is very close to theoretical results 1060 K given by Rosengaad and Johansson,[25] and 1095 K given by Uhl and Kübler.[24] It is interesting to note that although the Hamiltonian we adopted [i.e., Eq. (1)] is a simplified Heisenberg model which is certainly unable to describe all the detailed magnetic behaviors of the whole system, it seems reasonable enough to examine the thermal properties of such magnetic systems (even low-dimensional ones, see next paragraph). This is mainly because the bcc Fe-based systems are strong ferromagnetic ones free of any frustrations, and the finite temperature magnetism is determined dominantly by the small spin deviations around the ferromagnetic ground state.

By using T_c extracted from the U_L-T curve, the critical exponent β is also deduced from the slope of the $\ln(M/M_0)$ - $\ln(T_c-T)/T_c$ plot, where M_0 is the magnetization at 0 K. Because the value of β is very sensitive to T_c, we have made the calculated T points very dense when temperature approaches to T_c. The estimated β is 0.36 ± 0.02, which agrees well with 0.3646 of other theoretical calculation for three dimensional Heisenberg model[37] and is also close to 0.38 of experimental one.[36] This fact verifies our MC calculations with the Heisenberg model. Although quantum fluctuations are neglected which might be important at low temperature, the presently adopted classical Heisenberg model seems reasonable enough to describe the critical behaviors near T_c.

It is noted that the calculated T_c is always overestimated compared with the experimental one. The reason might comes from two aspects. The exchange integrals are esti-

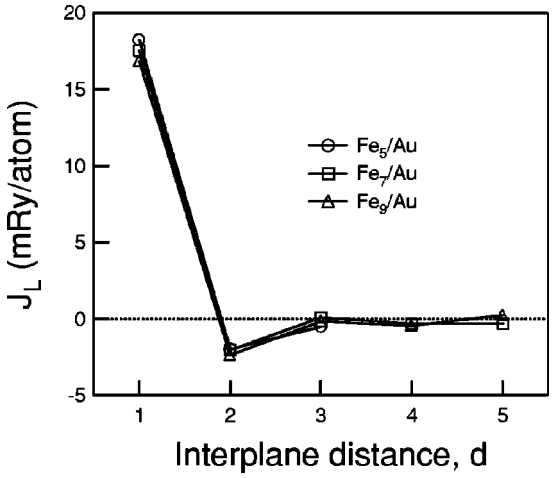

FIG. 1. Interlayer exchange parameter J_L as a function of the distance d ($d=|i-j|$) between the ith and jth Fe planes in the bcc-Fe/Au multilayers.

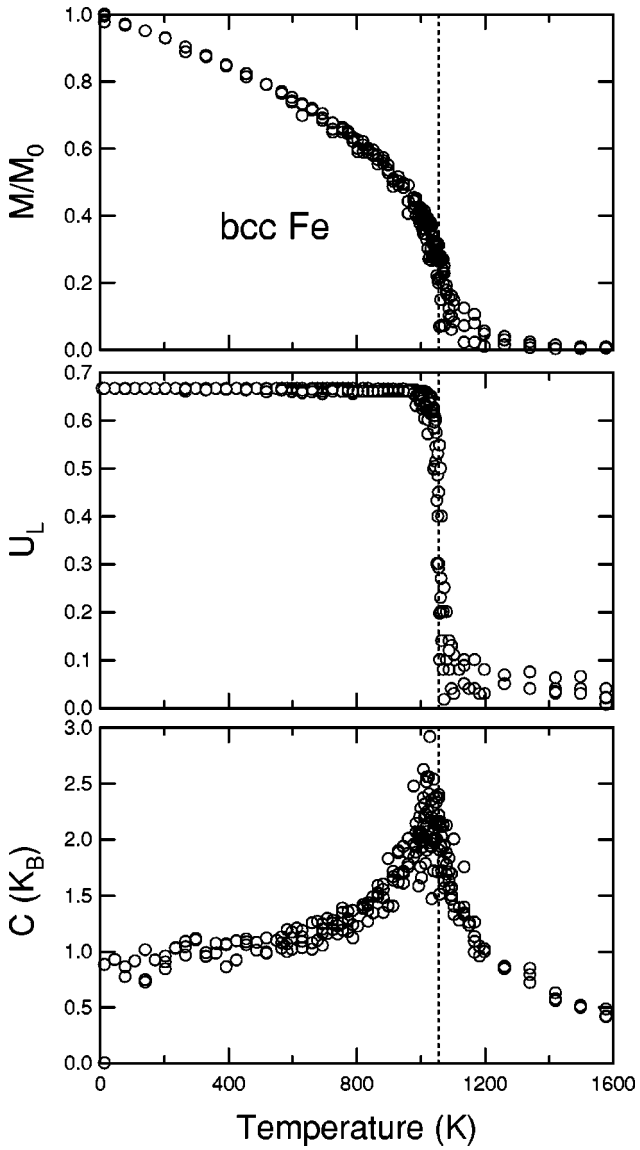

FIG. 2. Temperature dependence of the magnetization (M), the fourth-order cumulant (U_L), and the specific heat (C) for bcc Fe with system size $16\times16\times16$.

mated at zero temperature and are kept as constants when the temperature increases. However, in fact, when the temperature increases, on the one hand, the absolute value of the local magnetic moment should certainly decrease due to thermal fluctuations; on the other hand, the lattice is expanded so as to decrease further the overlap between two atoms. These two effects make the effective exchange integrals obtained at 0 K overestimated for the case when temperature approaches to T_c, which make the T_c overestimated always. A better theoretical approach would be to take such effects self-consistently into account. However, at the present stage limited by computational power, this seems rather unrealistic. Fortunately, such overestimation seems small because these two effects are very weak.

Encouraged by the good agreements achieved on the bulk Fe, we apply the same scheme to study the layered $Fe_n/Au(001)$ superlattices which are essentially quasi-2D systems. However, a naive application of the above developed method is not correct, since according to Mermin-Wagner theory,[38] there is no long range order established at finite-temperature for *isotropic* Heisenberg system with dimension lower than 3D. In real materials, because of the existence of the anisotropy, the magnetization is always stabilized.[2] Theoretically, Bander and Mills have demonstrated that a phase transition to ferromagnetism occurs always for arbitrarily small anisotropy for 2D system using the renormalization group scaling method;[39] Zhou *et al.*[40] have examined the finite-temperature magnetism of magnetic multilayers with magnetic anisotropy included in the Heisenberg model using Green's function technique. In the present work, to correctly study the phase transitions in such low-dimensional systems, we thus introduce a model anisotropy term $-D_K M_z^2$ to the Hamiltonian (1), where D_K is the anisotropy constant. However, it is still a challenging problem to get the accurate value of D_K from the first-principles, due to both technique (say, the extremely large number of k points required to achieve convergence) and even more fundamental reasons (a general discussion given by Gay and Richter in Ref. 1). Fortunately, it is demonstrated that T_c is only weakly dependent on the anisotropy constant D_K in bulk metals,[41] and later our calculation also shows that T_c is rather insensitive to D_K value in the experimentally permitted range. As an illustration, in Fig. 3, the magnetization (M), the fourth-order cumulant (U_L), and the specific heat (C) of Fe_2/Au_2 are plotted with D_K varying from 0.01 to 0.2 mRy/atom, which is a range large enough to cover all the experimental measurements ($\sim$0.04 mRy/atom, see Ref. 2). It is interesting to note that while this anisotropy essentially influence the value of the critical exponent β, it does not do so on the value of T_c in the calculated D_K range. This fact indicates that T_c is essentially determined by the exchange interactions, which can be accurately fixed by the *ab initio* calculations without SOC, so that the present *ab initio* MC method is possible to predict sensible T_c values for low-dimensional systems as well as bulk metals.

Based on the *ab initio* MC calculations, the Curie temperatures for all the systems considered here are obtained and then plotted in Fig. 4 as the functions of Fe layer thickness n. It is seen that T_c is a smooth increasing function of Fe layer thickness, which increases from 582–1057 K as the Fe layer thickness increases from 2 ML to bulk. Considering the possible numerical errors from the least-square fitting, the influences of the different D_K values, as well as the MC simulations themselves, the total inaccuracies of these calculated results are estimated to be ±30 K.

Recently, Riedling *et al.*[9] investigated the temperature dependence of the magnetization reversal process and the spin-waves in epitaxially grown (001)-oriented $[Fe_n/Au_m]_{30}$ multilayers ($n=1,\ 2;\ m=1-6$), and showed that T_c for Fe_2/Au_m ($m=1,\ 3,\ 5$) should be larger than 460 K. T_c in 2 ML ultrathin film is reported to be 467 K,[42] which is smaller than 582 K of the present theoretical result for Fe_2/Au_2 superlattice. However, the experimental reports on the accurate values of T_c for Fe_n/Au layered superlattices are still lacking. To our knowledge, this is the first time that theoretical estimations of T_c for low-dimensional systems which are closer to first principles have been presented.

Generally, according to Weiss' theory, T_c is proportional to the *effective* coordination number $z_{\rm eff}$ times the *renormalized* exchange coupling $J_{\rm eff}$ which implicitly includes the ef-

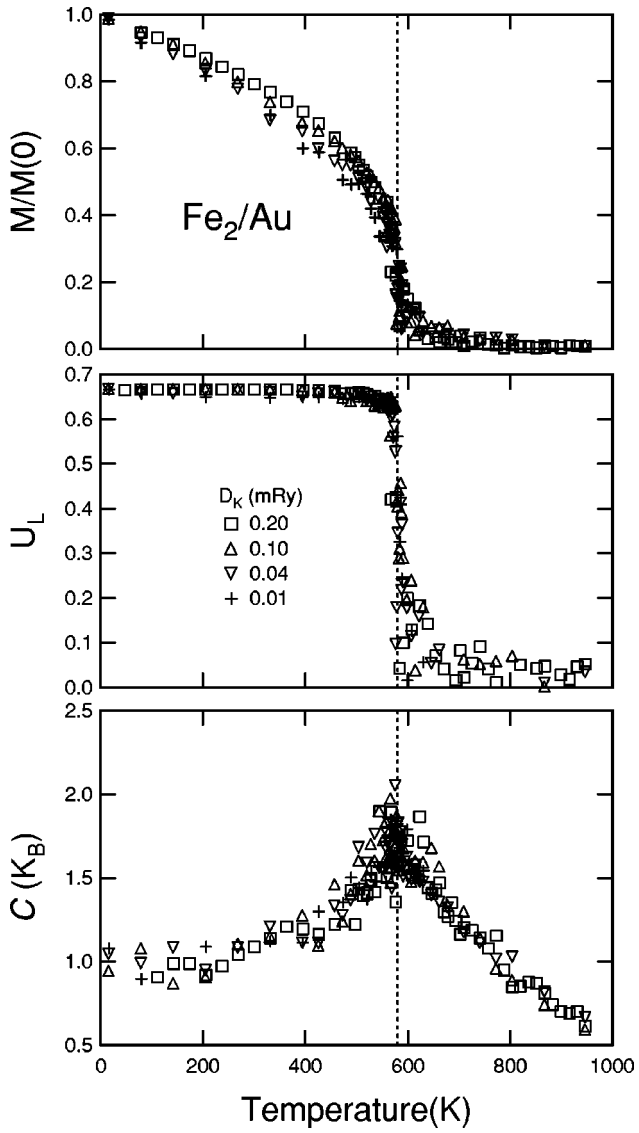

FIG. 3. Magnetization (M), fourth-order cumulant (U_L), and specific heat (C) for $Fe_2/Au(001)$ superlattice with system size $32\times32\times2$.

fects of the magnetic moments, namely, $T_c \sim z_{\text{eff}} J_{\text{eff}}$. To better understand the calculated results in the layered FeAu systems, let us make the assumption that J_{eff} is not drastically changed when the Fe layer thickness decreases (see Table II), then T_c should be proportional to z_{eff} directly. Thus, we have $T_c(n) = T_c^{\text{bulk}}(1-1/n)$ as a function of the Fe film thickness n, since the *effective coordination number* of Fe is $8-8/n$ in the layered bcc-$Fe_n/Au(001)$ superlattices. In Fig. 4, T_c estimated from the Weiss' law is also plotted (solid line) for comparison. It is shown that while the general behavior is essentially governed by Weiss' law, there is 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.[13]

On the other hand, some authors have employed an Ising model to study the finite-temperature magnetism in fcc-Fe/Cu systems.[43] We have also performed the MC simulations with the Ising model, and plotted the T_c in Fig. 4 for comparison. It is seen that the T_c values 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 for layered magnetic systems.

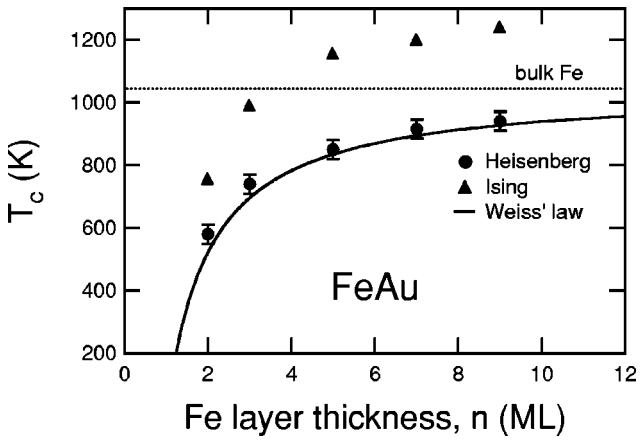

FIG. 4. Dependence of the Curie temperature on the Fe layer thickness (n). Solid circles indicates the Heisenberg-MC results, triangles indicates the Ising-MC ones. Solid line represent the Weiss' law expressed by $T_c(n) = T_c^{\text{bulk}}(1-1/n)$.

IV. SUMMARY

In summary, we have examined the exchange interactions of layered FeAu superlattices by using the self-consistent FLAPW method under the GGA. These superlattices are found to have ferromagnetic ground states with enhanced moments due to the interface effects. In addition, the Curie temperatures are estimated by using the MC simulations based on the Heisenberg model with *ab initio* exchange parameters and a phenomenological anisotropy constant. Numerical calculations demonstrate that the value of T_c is rather insensitive to the magnetic anisotropy in the experimentally permitted range, but is essentially determined by the exchange interactions which can be obtained from the *ab initio* calculations. T_c is found to be a smooth function of Fe layer thickness and decreases as decreasing of Fe layer thickness due to the reduced coordination number of Fe atoms at interfaces according to Weiss' law. However, interface effect contributes a nontrivial enhancement of T_c over the Weiss's law result. From the present study, it is shown that the *ab initio* Heisenberg MC method works well to describe the finite-temperature magnetism in the low-dimensional superlattices as well as in the bulk metals.

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