Electronic and magnetic structures of Fe/Cr/Fe sandwiches and Fe/Cr superlattices

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Realistic tight-binding band calculations have been performed for $(Fe)_3/(Cr)_m/(Fe)_3$ sandwiches and for $(Fe)_3/(Cr)_m$ superlattices by varying the number of Cr layers, $m=3$, 4, and 5. The distributions of local magnetic moments on Fe and Cr layers have been determined self-consistently. Similarities and differences between the calculated moment distributions in the sandwiches and the superlattices are discussed. The calculated Cr-thickness dependence of the interlayer exchange interactions in Fe/Cr superlattices is also reported. Our calculations account for the recently observed antiferromagnetic coupling between Fe layers across Cr layers in the Fe/Cr multilayers.

I. INTRODUCTION

Currently Fe/Cr multilayers have attracted much interest because of their unusual behavior.[1-9] It has been reported[1-4] that the total magnetic moments of successive Fe layers couple antiferromagnetically across interspacing Cr layers. They exhibit a large magnetoresistence depending on the relative orientation of magnetization.[4-7] Since the antiferromagnetic (AFM) coupling of Fe moments is expected to play an essential role in the observed large magnetoresistance,[8,9] it is indispensable to theoretically study the mechanism of these antiferromagnetic couplings. When we apply the localized (Heisenberg or Ising) model with nearest-neighbor interactions to the Fe/Cr superlattice, successive Fe layers align ferromagnetically or antiferromagnetically across the intervening Cr layers, depending on whether the number of Cr layers is odd or even;[10] the former (latter) configuration is referred to as the FM (AFM) solution hereafter. On the contrary, various experiments such as light scattering,[1,3] spin-polarized low-energy electron diffraction (LEED),[2] and magnetization measurements[3,4,7] show that this is not the case. Thus, the observed antiferromagnetic coupling cannot be explained with a simple localized model even if the roughness at the interfaces is taken into account.[3]

Fe and Cr atoms are typical transition metals in which d electrons have both the localized and itinerant characters. It is desirable to study the magnetic properties of Fe/Cr multilayers based on the itinerant-electron model rather than the localized model. Quite recently Levy *et al.*[9] made a detailed band calculation for $(Fe)_3/(Cr)_3$, $(Fe)_3/(Cr)_5$, and $(Fe)_4/(Cr)_4$ superlattices to show that the AFM solution can be more stable than the FM solution even when the number of Cr layers is odd.

Reported experiments have been performed mainly for Fe/Cr/Fe sandwiches which are epitaxially grown on nonmagnetic substrates. We expect that Fe/Cr/Fe sandwiches are physically similar to Fe/Cr superlattices, for which a band calculation has been made.[9] In a strict sense, however, the two systems are not equivalent. For example, superlattices have translational symmetry along the direction perpendicular to the interface but sandwiches do not. It is one of the purposes of the present paper to perform realistic tight-binding band calculations[11,12] for Fe/Cr superlattices and relevant sandwiches in order to examine the similarities and differences between the two systems.

The second purpose of this paper is to calculate the interlayer exchange interaction, J, in Fe/Cr superlattices. From the calculated energy difference between the FM and AFM solutions, Levy *et al.*[9] have estimated J to be of the order of 0.075 eV for the $(Fe)_3/(Cr)_5$ superlattice. However, their derivation of J from the calculated energy difference is not clear and their result is considered to be much overestimated compared with the experimental data.[9] In the present paper, we calculate the interlayer exchange interaction by using an alternative approach. We employ the analytical expression for J (Ref. 12) which is obtained by a perturbation calculation of the energy shift due to a magnetic-moment pair embedded in the paramagnetic Fe/Cr superlattice. As will be shown shortly, our approach yields the reasonable Cr-thickness dependence of the interlayer exchange interaction.

The outline of the present paper is as follows: In Sec. II we briefly describe the model and method of calculation[11,12] employed in this study. The calculated moment distributions in the sandwiches and superlattices are presented in Sec. III. We discuss, in Sec. IV, the interlayer exchange interaction in the Fe/Cr superlattice. Section V is devoted to conclusions.

II. MODEL AND METHOD OF CALCULATION

We employ the method of calculation for electronic structures of surfaces, sandwiches, and superlattices, which was developed by the present author.[11,12] We assume $(Fe)_3/(Cr)_m$ superlattices ($m=3$, 4, and 5), in which both Fe and Cr atoms lie on a common bcc lattice with [001] interfaces. As for sandwiches, we adopt $(Fe)_3/(Cr)_m/(Fe)_3$ layers ($m=3$, 4, and 5) sandwiched by Cu, which are put on Cu substrates with the bcc [001] surface. The configuration of the sandwiches is given as $(Cu)_3/(Fe)_3/(Cr)_m/(Fe)_3/(Cu)_3/Cu(001)$, Cu layers simulating nonmagnetic overlayers and substrates employed in the experiments. The layers parallel to the in-

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terface or the surface are assigned by the index n. We neglect the crystalline anisotropy to simplify our calculation, although it may play an important role. We employ the tight-binding Hamiltonian given by[11,12]

$$H = H_0 + H_I \ , \tag{1}$$

with

$$H_0 = \sum_{\sigma} \sum_{j} \sum_{m} E_j a^{\dagger}_{jm\sigma} a_{jm\sigma} + \sum_{\sigma} \sum_{j,j'} \sum_{m,m'} t^{mm'}_{jj'} a^{\dagger}_{jm\sigma} a_{j'm'\sigma} \ , \tag{2}$$

$$H_I = \tfrac{1}{4} \sum_{j} (U_j N_j^2 - J_j M_j^2) \ , \tag{3}$$

where $a^{\dagger}_{jm\sigma}$ ($a_{jm\sigma}$) is a creation (annihilation) operator of a σ spin electron of the orbital m on the lattice site j. The core potential, E_j, is assumed to be common for all orbitals. The two-center transfer integrals, $t_{jj'}$, are given by the canonical relation[13]

$$\left.\begin{matrix}(dd\sigma)\\(dd\pi)\\(dd\delta)\end{matrix}\right\} = \left\{\begin{matrix}-6\\4\\-1\end{matrix}\right\} \times (W_d/2.5)(S/R)^5 \ , \tag{4}$$

where R is the interatomic distance, $S=(3/16\pi)^{1/3}a$ is the Wigner-Seitz radius, a is the bcc lattice constant, and W_d is the bandwidth parameter. We adopt $W_d = 8.00$, 6.12, and 4.08 eV for Cr, Fe, and Cu, respectively.[13] The transfer integrals are included up to the second-nearest neighbors. As for the transfer integrals between Fe-Cr (Fe-Cu) pairs, we employ the geometrical averages of the values of Fe-Fe and Cr-Cr (Cu-Cu) pairs.[13] In Eq. (3), N_j (M_j) denotes the total charge (magnetic-moment) operator at the site j, and U_j and J_j are Coulomb and exchange interactions, respectively. To reduce the number of parameters, we assume $U_j = J_j$, which are treated within the Hartree-Fock approximation.[11,12] The U_j values for Fe and Cr are chosen such that we obtain the ferromagnetic ground state in bulk Fe with the magnetic moment of $2.2\mu_B$ and the commensurate antiferromagnetic state in bulk Cr with the sublattice moment of $0.6\mu_B$. Our result for Fe is consistent with experiments[14] and the band calculations using the local-spin-density-functional (LSDF) method.[15] Since our Cr result refers to a commensurate antiferromagnetic state, it should be compared with the observed maximum value of the spin-density wave (SDW) of $0.59\mu_B$.[16] Our Cr result is also consistent with some recent LSDF band calculations for the commensurate SDW,[17,18] although smaller sublattice moments are reported in other calculations.[19,20] We assume the U value for Cu to be the same as that for Fe although a change of its value hardly modifies the calculated results because Cu is nonmagnetic. The number of d electrons in Cr, Fe, and Cu are taken as 5.0, 7.4, and 10.0 electrons per atom, respectively.[13] The core potentials, E_j, for Fe and Cr are chosen to preserve the local charge neutrality, neglecting slight deviations (less than 0.1 electrons/atom) at interfaces. From separate calculations for pure Fe and Cu, the core-potential difference between Fe and Cu is taken as $E_{\mathrm{Cu}} - E_{\mathrm{Fe}} = -3.8$ eV, although the calculated results are insensitive to a choice of E_{Cu}.

III. CALCULATED RESULTS

Numerical calculations were performed for the sandwiches and superlattices by using the same band parameters summarized in Table I (details of the method of calculation have been explained in Refs. 11 and 12). We assumed that all atoms on a given nth layer have the same averages of local moments and number of electrons, M_n and N_n, which were calculated self-consistently by an iterative method. Our calculation was started with trial values of M_n and N_n, from which their new averages were obtained. The iteration was continued until the new results agreed with the old ones within the assumed accuracy of 0.025 electrons/atom (μ_B/atom). Our computer program looks for a solution which is locally stable in the configuration space. Iterative calculations were repeated by adopting a variety of initial, trial solutions.

A. Fe/Cr/Fe sandwiches

First we discuss the results for the $(\mathrm{Fe})_3/(\mathrm{Cr})_m/(\mathrm{Fe})_3$ sandwiches in which we obtained the FM and AFM solutions, both of which are numerically stable. Figures 1(a) and 1(b) show the calculated results of the AFM and FM solutions, respectively. Details of the calculated local moments on the nth layer, M_n, for $m=4$ and 5 are shown in Figs. 2 and 3, respectively. The profiles of the calculated moment distributions are almost completely symmetric or antisymmetric with respect to the center of the sandwiches. The substrate Cu layers have no local moments. The Cu interfaces are slightly polarized because of the molecular field arising from adjacent Fe layers. The calculated moment distributions on Fe and Cr layers have the following features.

(i) Magnetic moments at the central Fe layers are $2.5\mu_B$, which are larger than the bulk value of $2.2\mu_B$. Fe atoms at the interfaces adjacent to Cr layers have moments of $1.5\mu_B$ while those near Cu layers have moments of $2.2\mu_B$. The difference between Fe moments in the FM and AFM solutions is very small.

(ii) Magnitudes of Cr moments in the FM solutions for $m=3$ and 5 and in the AFM solution for $m=4$ are about $1.0\mu_B$, which are enhanced compared to the bulk value of $0.6\mu_B$. In other cases, Cr atoms have much smaller moments.

(iii) The moment distribution of the AFM solution for odd m ($=3$ or 5) has a node at the central Cr layer.

(iv) The coupling between Fe and Cr moments at the interfaces is antiferromagnetic both in the AFM and FM solutions.

The enhanced moments on Fe and Cr layers are attributed to the two-dimensional character of the sandwiches. It has been reported that Fe moments in

TABLE I. Parameters (in eV) used in the calculation.

	E_n	W_d	U_n
Cr	0.00	8.00	0.67
Fe	−2.00	6.12	0.80
Cu	−5.80	4.08	0.80

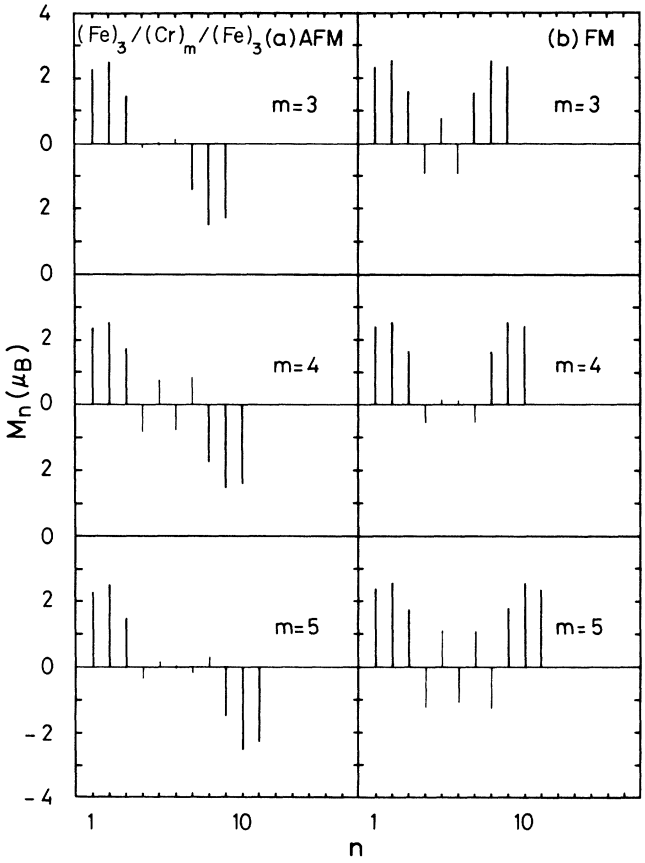

FIG. 1. Magnetic-moment distribution against the layer index n of (a) AFM and (b) FM solutions in the $(Fe)_3/(Cr)_m/(Fe)_3$ sandwiches ($m=3$, 4, and 5), local moments on Fe and Cr layers being expressed by bold and thin solid lines, respectively.

Cu/Fe/Cu(001) are $(2.3-2.7)\mu_B$ (Ref. 21) and that a Cr moment sandwiched by Au has a giant moment of 3.1 μ_B.[22]

B. Fe/Cr superlattices

Next we discuss the calculated result of the superlattices. For a given $(Fe)_3/(Cr)_m$ superlattice, we again obtained both the FM and AFM solutions. The calculated moment distributions in the FM and AFM solutions are shown in Figs. 4(a) and 4(b), respectively. Figures 5 and 6 show details of the local moments in $(Fe)_3/(Cr)_4$ and $(Fe)_3/(Cr)_5$ superlattices, respectively. In both the FM and AFM solutions, magnetic moments at the central Fe layers are $2.5\mu_B$ while those at the interface Fe layers are

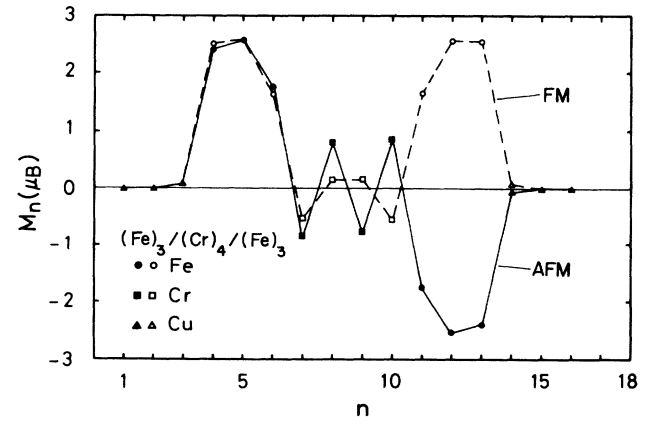

FIG. 2. Local moments in the AFM (solid curve) and FM (dashed curve) solutions in the $(Fe)_3/(Cr)_4/(Fe)_3$ sandwich.

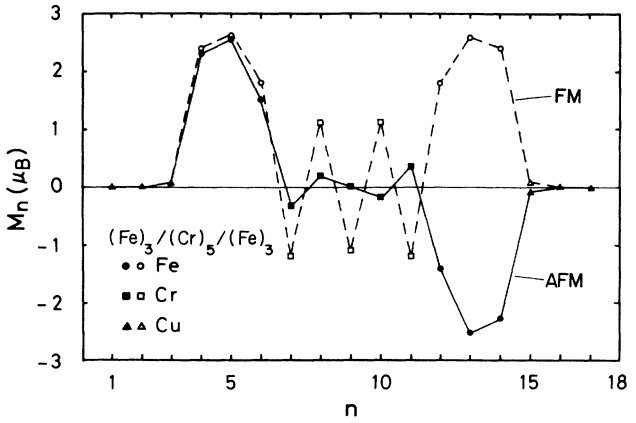

FIG. 3. Local moments in the AFM (solid curve) and FM (dashed curve) solutions in the $(Fe)_3/(Cr)_5/(Fe)_3$ sandwich.

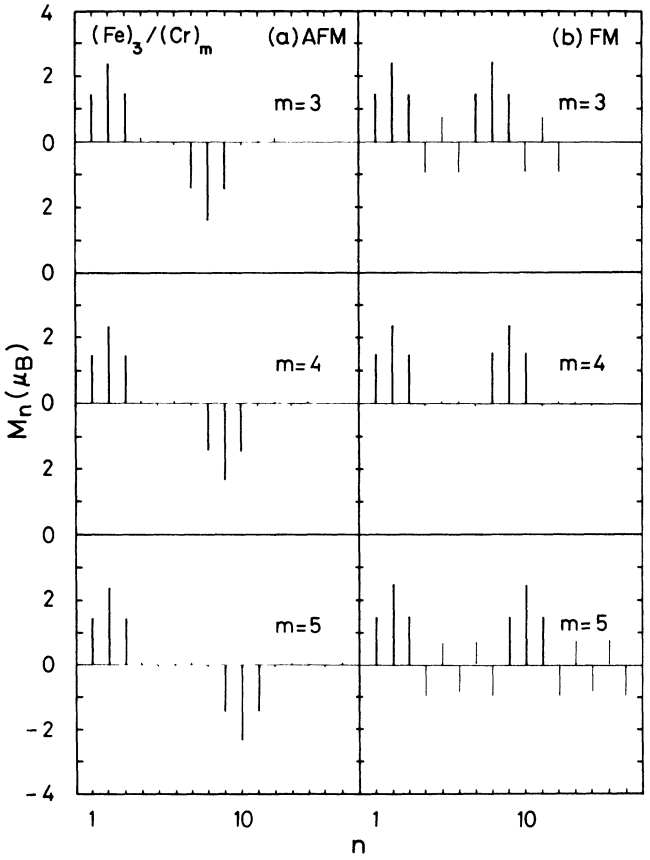

FIG. 4. Magnetic-moment distributions in the magnetic unit cell of (a) AFM and (b) FM solutions in the $(Fe)_3/(Cr)_m$ superlattices ($m=3$, 4, and 5), local moments on Fe and Cr layers being expressed by bold and thin solid lines, respectively.

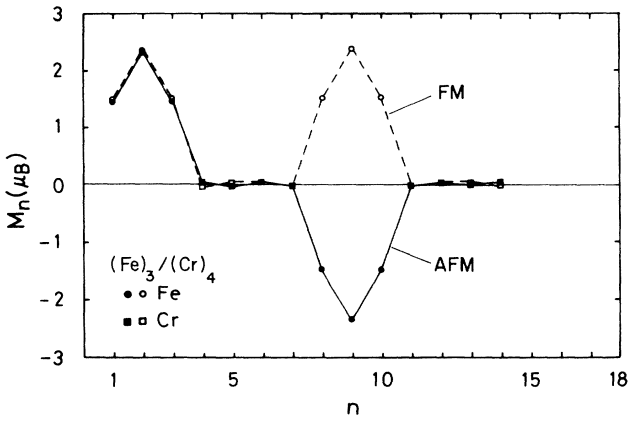

FIG. 5. Local moments in the magnetic unit cell of the AFM (solid curve) and FM (dashed curve) solutions in the $(Fe)_3/(Cr)_4$ superlattice.

$1.4\mu_B$. On the contrary, the Cr moments depend sensitively on the type of solutions (FM or AFM) and the number of Cr layers. In the FM solution for $m=3$ or 5, Cr atoms have moments of about $0.8-1.0\mu_B$, which are larger than $0.6\mu_B$ of bulk Cr. However, Cr moments in the FM solution for $m=4$ are almost vanishing. In the AFM solution Cr moments are much smaller than those in the FM solutions. Particularly in the case of odd m ($=3$ or 5), the moment distribution has a node at the central Cr layer. Our results for $m=3$ and 5 are in good agreement with those of first-principles calculations made by Levy *et al.*[9]

The moment distribution in the Fe/Cr superlattices is almost the same as in the Fe/Cr/Fe sandwiches, except for the AFM solution with $m=4$; Cr moments in the former are nearly vanishing while those in the latter are about $0.8\mu_B$. This difference is expected to arise from the fact that Cr atoms locate near the critical condition for the appearance of magnetic moments and that the magnitude of Cr moments sensitively depends on the parameters and structures (e.g., sandwich or superlattice) employed in the calculation. In fact, even for *bulk* Cr, the

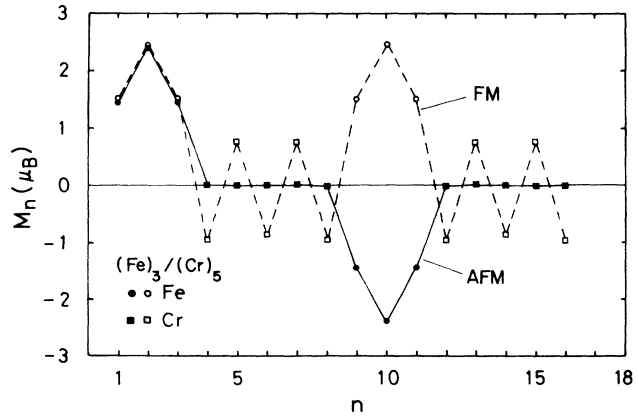

FIG. 6. Local moments in the magnetic unit cell of the AFM (solid curve) and FM (dashed curve) solutions in the $(Fe)_3/(Cr)_5$ superlattice.

sublattice moments previously calculated[17–20] do not agree due to a slight difference in the adopted schemes of the LSDF method.

Levy *et al.*[9] have claimed that when an alignment of the Fe moment is incompatible with the SDW in Cr, the Fe/Cr superlattice minimizes its total energy by *quenching* Cr moments. This is also actually realized in our Fe/Cr superlattices and Fe/Cr/Fe sandwiches. The cost of energy due to unfavorable moment alignments in the FM solution for even m or in the AFM solution for odd m, is compensated generally by *changing* the magnitudes of moments on Cr layers.[23] A node on the central Cr layer in the moment distribution in both the superlattice and sandwich has an ostensive similarity to the SDW in bulk Cr which has nodes with the period of about 21 layers in the [001], or its equivalent, directions.[16] Although the detailed mechanism of the SDW is different from that of our moment distribution with nodes, both phenomena arise from the itinerant character of Cr atoms in which the local moment may change its magnitudes.[23]

In order to establish which of the FM and AFM solutions is more numerically stable, it is necessary to calculate their ground-state energies. Levy *et al.*[9] have shown from the ground-state energy calculation that the AFM solutions may be more stable than the FM solution even when the number of Cr layers is odd. We have tried to calculate the total energies of our AFM and FM solutions. Unfortunately, we could not determine the definite value of the total-energy difference between the two solutions because it is comparable to, or smaller than, the numerical uncertainty in our calculation. An improvement of the calculation accuracy requires finer meshes in the energy integration and in the surface wave-vector samplings, and then much more computation time. In order to bypass this difficulty,[24] we calculated the interlayer exchange interactions in Fe/Cr superlattices. This quantity provides us with a clear physical insight into understanding the observed antiferromagnetic coupling of Fe layers, as will be discussed in the next section.

IV. INTERLAYER EXCHANGE INTERACTIONS

We assume the paramagnetic $(Fe)_1/(Cr)_m$ superlattice, in which a *pair* of local moments, M_n and $M_{n'}$, is embedded at lattice sites on the nth and n'th layers. The difference between the total energies when M_n and $M_{n'}$ are parallel ($E_{nn'}^{\uparrow\uparrow}$) and antiparallel ($E_{nn'}^{\uparrow\downarrow}$), is given up to the second order of M_n by[12]

$$E_{nn'}^{\uparrow\downarrow}-E_{nn'}^{\uparrow\uparrow}=2J_{nn'}M_nM_{n'}\ , \tag{5}$$

where $J_{nn'}$ is the interlayer exchange interaction between the nth and n'th layers given by

$$J_{nn'}=U_nU_{n'}\int d\varepsilon\, f(\varepsilon)\sum_{\sigma}(1/\pi)\mathrm{Im\,Tr}G_{nn'\sigma}G_{n'n\sigma}\ . \tag{6}$$

Here $f(\varepsilon)$ is the Fermi distribution function, Tr stands for the trace over the orbitals, and $G_{nn'\sigma}$ is the Green-function matrix. By using Eq. (6), we calculated the nearest-neighbor exchange interactions $J_{nn'}$ ($n'=n+1$) in bulk Fe and Cr, which are 0.069 and -0.059 eV, respectively. The sign of the nearest-neighbor exchange in-

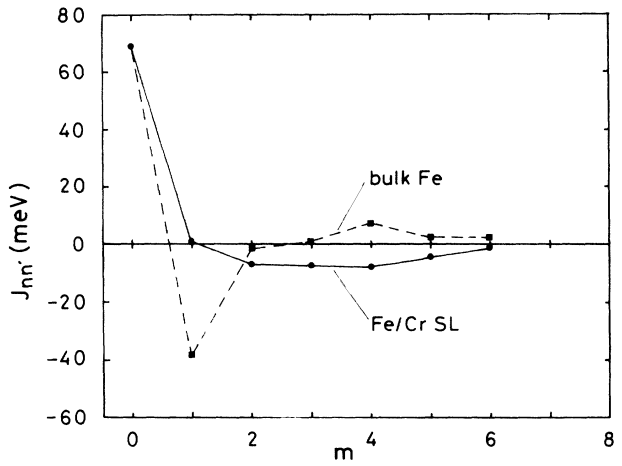

FIG. 7. The interlayer exchange interaction $J_{nn'}$ ($n'=n+m+1$) for a Fe-Fe pair as a function of m, the number of interspacing layers, in Fe/$(Cr)_m$ superlattices (SL) (solid curve) and in bulk Fe (dashed curve) (Ref. 25). The systems are assumed to be in the paramagnetic state.

teractions for a Fe-Fe pair is positive and that for a Cr-Cr pair is negative, as expected. We show, by the solid curve in Fig. 7, the calculated exchange interaction for a Fe-Fe pair in the $(Fe)_1/(Cr)_m$ superlattice as a function of m, the number of the interspacing Cr layers.[25] The exchange interaction is positive for the nearest-neighbor Fe-Fe pair ($m=0$) as mentioned above. It is nearly vanishing at $m=1$, and at $m>1$ the sign of $J_{nn'}$ is negative, which suggests that the AFM solution becomes more stable than the FM solution. The absolute value of $J_{nn'}$ has a maximum of 8 meV at $m\sim4$. We should note that this maximum in $|J_{nn'}|$ arises from the fact that the Fe-Fe exchange interaction is positive for a nearest-neighbor pair while for far-neighboring pairs it has a negative value with a monotonic decrease in its magnitude. For a comparison, we calculated the spacial dependence of the exchange interaction in bulk Fe, whose result is shown by the dashed curve in Fig. 7. It is positive at $m=0$, but negative at $m=1$, showing the oscillatory behavior. This is consistent with the previous calculations for bulk Fe.[26-28]

It has been reported[1-4,7] that, when the Cr thickness, t_{Cr} is changed, the effective exchange coupling between Fe layers varies from ferromagnetic at $t_{Cr}<t_c$ to antiferromagnetic at $t_c<t_{Cr}<t_m$. Here the critical thickness t_c depends on the experimental conditions; $t_c\sim5$ Å (Ref. 3) or 12 Å (Ref. 7) and t_m is of the order of 20 Å. Nguyen *et al.*[4] obtained a monotonic decrease in J as t_{Cr} increases at 9 Å $<t_{Cr}<30$ Å. On the contrary, Krebs *et al.*[7] reported the J dependence with a peak at $t_{Cr}\sim16$ Å. Quite recently Parkin *et al.*[29] have shown that the magnitude of J oscillates with t_{Cr} with a periodicity of about 18–20 Å, similar to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.[30] Although the experimental data reported so far are still conflicting in the behavior of J, its general trend for $t_{Cr}<t_m$ is well explained by our calculation, at least in the qualitative sense.

V. CONCLUSIONS

We have calculated the electronic and magnetic structures of thin Fe/Cr/Fe sandwiches and Fe/Cr superlattices by using the realistic tight-binding model.[11,12] Our calculations[24] have shown that the antiferromagnetic alignments of Fe layers may be favorable in the superlattice and sandwiches, which is in accordance with the recent experiments.[1-4,7] This arises from the itinerant character of Cr atoms[23] and cannot be realized in the localized model even if the long-range interactions are included. The existing theories[8,9] explaining the observed large magnetoresistance[4-7] assume the absence of magnetic moments on Cr layers in the Fe/Cr multilayers. It might be possible that Cr moments, which are enhanced ($\sim1.0\mu_B$) because of the two-dimensional character of the Fe/Cr multilayer, play important roles in the scattering process of electron conduction. In order to make a more precise comparison with the experimental data, we are now under consideration to extend our calculation to thicker sandwiches. This is feasible because the computation time is proportional to the thickness of the sandwich, while in the superlattice the CPU time is exponentially increased as the size of its magnetic unit cell becomes large. It would be also interesting to make a theoretical study on finite-temperature properties of Fe/Cr sandwiches and superlattices.

ACKNOWLEDGMENTS

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[23]Although magnitudes of local moments are fixed in the localized model, the itinerant model has an extra degree of freedom varying them depending on the environment.
[24]We have confirmed that the AFM solution is the stable ground state in our Fe/Cr/Fe sandwiches and Fe/Cr superlattices from a calculation of $\phi_n(\zeta_n)$. It expresses the local energy when a *single* atom with a moment of ζ_n is embedded as an impurity at a given site on the nth layer in an otherwise pure system [its explicit expression has been given, for example, in Eq. (2.13) of Ref. 12]. This quantity has been calculated in conjunction with the study on finite-temperature properties of the Fe/Cr multilayers. The difference, $\phi_n(\zeta_n)-\phi_n(M_n)$, denotes the energy shift when the value of the ground-state moment at the given site on the nth layer, M_n, is changed to ζ_n. We have obtained that the relation $\phi_n(\zeta_n)>\phi_n(M_n)$ holes for $\zeta_n \neq M_n$ in the AFM solutions.
[25]The interlayer exchange interactions for $m=0$, 1, 2, 3, 4, 5, and 6 along the [001] direction correspond to the first-, second-, fourth-, sixth-, tenth-, thirteenth-, and eighteenth-neighbor interactions, respectively, in the bcc lattice.
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