Oscillatory exchange coupling between iron layers separated by chromium

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The exchange coupling J between Fe layers separated by nonmagnetic Cr is calculated for Fe/Cr/Fe (001) trilayer structures as a function of the spacer thickness N for several temperatures T. It is shown that for perfectly sharp interfaces $J(N,T)$ is entirely dominated by short period oscillations for $0\ \mathrm{K} \leqslant T \leqslant 500\ \mathrm{K}$ and N varying from 5 to 50 atomic planes. At zero temperature the amplitude of J decays as $N^{-3/2}$ for large values of N. This behavior is caused by the particular type of singularity in the nesting of the Cr Fermi which is responsible for one of the dominant short-period oscillations of $J(N)$. A strong temperature dependence of the coupling strength is obtained for some values of N, in excellent agreement with experiments. The effect of interface mixing on $J(N)$ reduces the overall coupling strength, as well as the relative importance of the short period oscillatory components, and causes a phase shift in the oscillations of $J(N)$. [S0163-1829(99)03317-2]

I. INTRODUCTION

Fe/Cr systems have been at the forefront of research in magnetic multilayers in recent years. About a decade ago it was observed that the exchange coupling J between Fe layers separated by Cr changes sign for different Cr thicknesses.[1] Later, it was found that J generally oscillates as a function of the spacer thickness N in metallic multilayers.[2] The rather large period of ≈ 18 Å observed in early measurements of $J(N)$ in Fe/Cr caused surprise and greatly stimulated the development of theories and experiments.[3–7] In addition, the striking ''giant'' magnetoresistance effect was discovered in Fe/Cr multilayers.[8] The importance of interface quality and crystal ordering of the intervening layer in highlighting different periods of $J(N)$ was experimentally evidenced in Fe/Cr/Fe wedge structures.[9–11] Some of the earliest observations of noncollinear spin structures corresponding to 90° coupling of the magnetic layers were made on Fe/Cr/Fe sandwiches,[12–14] and the search for the physical origin and relative importance of this type of coupling in different systems has further stimulated theories and experiments.[15,16]

It is well known that the magnetic ground state of Cr is rather delicate. Bulk Cr exhibits a spin-density-wave (SDW) antiferromagnetism, which is not commensurate with its lattice. The SDW in Cr originates from Fermi-surface nesting, which causes a maximum in the noninteracting static spin susceptibility at a wave vector close to $2\pi/a$, where a is the Cr lattice constant. Such nesting can be modified by alloying Cr with different materials, in some cases drastically affecting its Néel temperature $T_N \sim 311$ K.[17] The presence of the Fe layers in Fe/Cr/Fe (001) trilayers poses magnetic boundary conditions which affect both the magnetic state and T_N of the Cr layer. Interfacial inhomogeneities can also largely affect J and the magnetic properties of the Cr spacer layer, especially for small Cr thicknesses.[15,18–21] For sufficiently thick Cr layers the SDW is likely to settle. However, long-range magnetic order may be suppressed in relatively thin Cr layers, due to frustrations generated by the presence of roughness, interdiffusion, vacancies, and steps at the Fe/Cr interface.[19,20,22,23]

In spite of the remarkable progress made in our understanding of the interlayer coupling in Fe/Cr systems, there are still several aspects which deserve clarification. In many Fe/Cr specimens, it has been observed that $J(N)$ oscillates basically with a long period, having maximum antiferromagnetic (AF) amplitude ≈ 1 mJ/m^2. Short-period oscillations of ≈ 2 monolayers are seen only in carefully grown samples.[9,24–26] On the other hand, all existing calculations assuming perfect interfaces find that $J(N)$ in Fe/Cr/Fe (001) trilayers is dominated by the short-period oscillations. Additionally, the coupling amplitude calculated across AF Cr invariably comes out much larger than that mediated by nonmagnetic Cr, and the latter is, in turn, much larger than those measured so far.[19,27,28] These discrepancies are rightfully attributed to interface inhomogeneities and lack of crystal ordering in the spacer. Experimentally it has been recognized that interface mixing always occurs even in the best-grown Fe/Cr samples. Its amount and extent depend on the substrate temperature during growth, and are difficult to be accurately determined.[21,29]

There are general rules which provide a systematic way of determining the oscillation periods of $J(N)$ for sufficiently large spacer thicknesses. According to Ruderman-Kittel-Kasuya-Yosida (RKKY)-like theories they are given by the extremal spanning vectors of the spacer Fermi surface (FS).[30,31] Quantum-well theory, however, predicts additional possibilities, especially when the spacer FS has more than one sheet,[32] as in the case of Cr. Because of the complexity of its FS, a complete analysis of all possible individual components of the coupling mediated by Cr is rather involved. First, because of the large number of Cr FS extrema. Second, one would need investigate the possibility of occurrence of non-RKKY contributions, coming from critical points associated with integer linear combinations of the various Cr FS sheets. Besides, for those extrema associated with nesting between different bands, the stationary phase approximation, usually employed in this type of analysis, is somewhat subtler, and in some cases not applicable.[32]

Contributions coming from several extremal points of the Cr FS have been calculated.[33,34] Nevertheless, the determination of the most important periodic components of $J(N)$ in Fe/Cr/Fe trilayers has not been fully settled. The origin of the

18 Å period has been the subject of recent theoretical debate. There are strong arguments indicating that it comes from extremal dimensions associated with the N-centered ellipsoids of the Cr FS.[33,34] However, since its amplitude is so much smaller than those of the short-period contributions, one is led to ask: why does it experimentally dominate the coupling in so many different samples? What kind of inhomogeneity and how much of it would be required to suppress the short-period oscillations so that only a long period is observed? Another conjecture is related to the fact that, in principle, each oscillatory component of J behaves differently with temperature.[35,36] Would it be possible that in the case of Fe/Cr temperature effects could suppress the short-period components, revealing others with smaller amplitudes? To help answering such questions it is necessary to calculate $J(N,T)$ in these systems.

For spacers with relatively simple Fermi surfaces, the quantum-well theory predicts that the contributions to $J(N,T)$ coming from single point singularities (s) of the spacer FS are asymptotically (i.e., for $N \gg 1$) given by[35]

$$J(N,T)=\sum_s \frac{A_s k_B T \sin(\omega_s N+\phi_s)}{N \sinh[k_B T(B_s N+C_s)]}. \tag{1}$$

At $T=0$ it reduces to

$$J(N)=\sum_s A_s \sin(\omega_s N+\phi_s)/(B_s N^2+C_s N), \tag{2}$$

where N is the spacer thickness measured in number of atomic planes. B_s and ω_s depend only on geometrical aspects of the spacer FS around those singularities; i.e., on the FS velocities and extremal radii along the direction perpendicular to the layers, respectively. On the other hand, A_s, ϕ_s, and C_s depend also on the degree of confinement of the carriers in the spacer caused by the magnetic layers, hence, on the matching of the electronic states across the interfaces. Asymptotic expressions similar to Eqs. (1) and (2) have been extensively used to analyze both theoretical and experimental results for $J(N,T)$. However, it is noteworthy that approaches which rely on fits to results of numerical calculations or to experimental values of the coupling to obtain periods, amplitudes, phases, and decay rates of $J(N,T)$ must be viewed with caution for the following reasons: the expected asymptotic regime $\propto 1/N^2$, obtained from isolated FS singularities, applies solely to zero temperature, ordered spacers, and depending on the values of C_s, it sets in only for relatively large values of N ($N>20$–30 atomic planes at least). At finite T, the envelope functions of the oscillatory components vary exponentially with N. For Co/Cu/Co(001) trilayers at room temperature, for instance, there is no range of N in which the coupling amplitude can be correctly described by a dependence $\propto 1/N^2$.[35–37] Furthermore, these fittings usually involve several parameters and, in some cases, they are not unique.

For spacers with more complicated Fermi surfaces, such as Cr, where nesting between sheets occurs, the asymptotic decay of $J(N)$ may be different from the usual $1/N^2$ behavior, depending on the nature of the dominant singularity.[31] As discussed in Ref. 31, the expected rate of decay is $\propto 1/N$ for the extreme case of perfect planar nesting, and $\propto 1/N^{3/2}$ when a line of coincidence occurs. Therefore, it is necessary to know what the real asymptotic behavior of $J(N,T)$ is in Fe/Cr, and beyond what value of N it actually sets in, before one can use equations such as Eqs. (1) or (2) to analyze the data.

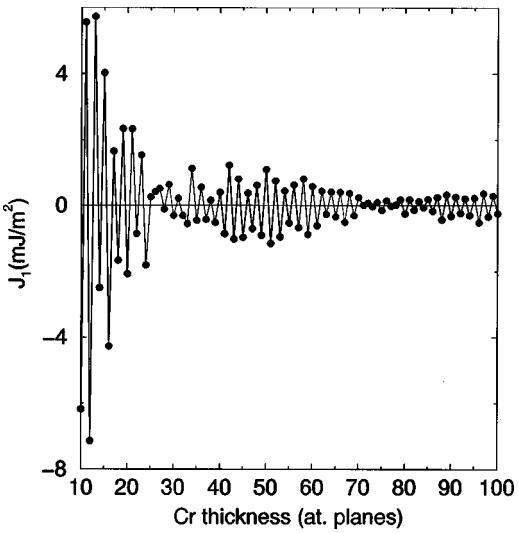

FIG. 1. Calculated exchange coupling at $T=0$ K for a Fe/Cr/Fe (001) trilayer as a function of the number of Cr atomic planes.

In this paper we show that for perfectly sharp interfaces, and at $T=0$ K, the amplitude of the coupling between Fe layers across noninteracting Cr, in Fe/Cr/Fe(001) trilayers, decays as $N^{-3/2}$ for large values of N. The asymptotic behavior of $J(N)$ sets in only for rather large Cr layer thicknesses: $N>30$ atomic planes. Therefore, the use of Eqs. (1) or (2) to analyze numerical or experimental values of the coupling for smaller Cr thicknesses is, strictly speaking, incorrect. We have also calculated $J(N,T)$ for several temperatures, and have found that for perfect interfaces it oscillates as a function of N with short-period oscillations for all temperatures investigated. For some values of N a strong temperature dependence of the coupling strength is obtained in excellent agreement with experiments. The effect of Fe/Cr interfacial mixing has also been investigated, and we show that for sufficiently large mixing the short-period oscillations tend to be suppressed and the long period begins to show up as expected.

II. RESULTS FOR PERFECT INTERFACES

We have used the formalism developed in Refs. 7 and 35 to calculate $J(N,T)$, defined as the total-energy difference per surface atom between the antiferromagnetic and ferromagnetic configurations of the trilayer. We show results for the bilinear exchange coupling term $J_1(N,T)$ which, for perfectly smooth Fe/Cr(001) interfaces, is virtually equal to $J/2$.[7] To calculate J we have used a tight-binding model with s,p,d orbitals, and hopping up to second-nearest neighbors. The tight-binding parameters for noninteracting Cr were taken from Ref. 38, and those for ferromagnetic Fe were obtained as in Ref. 39.

Results for $J_1(N,T=0)$ in Fe/Cr/Fe(001) trilayers are shown in Fig. 1. It is evident that short-period oscillations

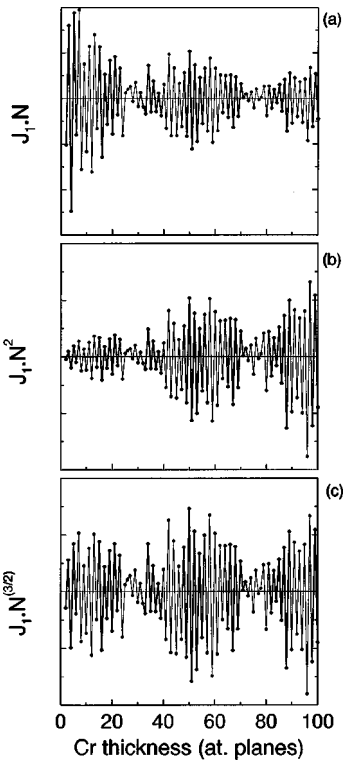

FIG. 2. Dependences of $J_1(N)\times N$ (a), $J_1(N)\times N^2$ (b), and $J_1(N)\times N^{3/2}$ (c), on the number N of Cr atomic planes. J_1 has been calculated at zero temperature, and is measured in mRy/surface atom.

dominate the calculated coupling at zero temperature for all values of N. Our values agree very well with those obtained in Ref. 28 for $N<20$ atomic planes, but they are 20–60 times larger than the experimentally observed first AF peaks. It is noteworthy that the coupling calculated across interacting Cr is even larger.[28,19] On the other hand, curiously, the maximum coupling amplitude measured in good-quality samples showing short-period oscillations is ≈ 3 times smaller than that observed in specimens where only a long period is apparent.[24] For thin Cr spacers the observed short oscillations show up superimposed to the long-period oscillation, suggesting that some degree of interfacial disorder is still present in those samples.

Before discussing the possible reasons for these disagreements between theory and experiments, we first address the question of how the coupling across noninteracting Cr really behaves asymptotically. To determine the correct asymptotic behavior of $J_1(N,0)$ we have calculated the coupling for large values of N, and plotted $J_1(N)\times N$, $J_1(N)\times N^2$, and $J_1(N)\times N^{3/2}$ as functions of N. It is clear from Fig. 2 that, at $T=0$ K, the oscillatory coupling across noninteracting Cr in Fe/Cr/Fe(001) trilayers decays asymptotically as $N^{-3/2}$, rather than N^{-2} or N^{-1} as assumed earlier.[28,27,40] The possibility of finding a $N^{-3/2}$ decaying rate has been envisaged by Koelling, provided the dominant contribution to J comes from a particular type of nesting where a line of coincidence occurs.[31] Below, we shall show that this is precisely what happens in noninteracting Cr. Before doing so, since we know the asymptotic behavior of J_1 we can estimate the relative amplitude of its most important oscillatory components, by taking the discrete Fourier transform[41] of $N^{3/2}J_1$ for large values of N. The result is shown in Fig. 3, and it clearly demonstrates that, asymptotically, J_1 is dominated mainly by three periods which are identified by the major peaks in the figure. Short-period oscillations are the most important ones. They come from the same FS nestings that cause the SDW in Cr, involving the electron and hole octahedralike FS pieces centered around the Γ and H points of the bcc Brillouin zone, respectively. Normally, such nesting is described as perfectly planar, but this is clearly an approximation. In fact, by observing it along the (001) direction, one realizes that it has critical points in the lines $k_x=\pm k_y$, $k_y=0$, and $k_x=0$, where x, y, and z are the usual cubic directions. The critical points located in the lines $k_x=\pm k_y$ are maxima, and those located in $k_y=0$, and in $k_x=0$ are minima. These stationary points are responsible for the short-period oscillations in $J(N,T)$; the maxima and the minima lead to oscillatory components of $J(N)$ having periods of ≈ 2.05, and 2.01 atomic planes, respectively.

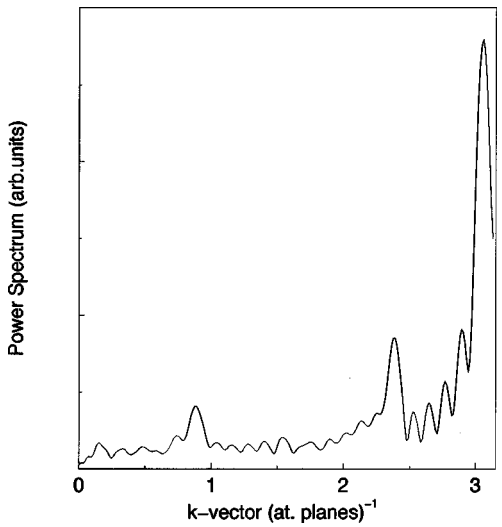

FIG. 3. Discrete Fourier transform of $N^{3/2}J_1(N)$ for $50\leqslant N \leqslant 100$, showing the periods of the most important oscillatory components of J_1.

A revealing result is shown in Fig. 4 where the calculated nesting surface is depicted around its critical points in order to determine the character of each singularity. The maximum leads to a contribution which, at $T=0$ K, has the usual N^{-2} asymptotic behavior. On the other hand, it is clear from Fig. 4(b), that the minimum associated with the nesting singularity at $k_y=0$ is extremely shallow along one of the principal axis directions. As a result, the corresponding effective mass is nearly infinite, thereby justifying the $N^{-3/2}$ asymptotic decay rate found in Fig. 2. We notice in Fig. 2(c), however, that the envelope bound of the first group of oscillations is clearly smaller than the asymptotic limiting value. This means that the asymptotic dependence $\propto 1/N^{3/2}$ is reached for Cr thicknesses >30 atomic planes. Consequently, in practice, this dependence may not be observed, because the SDW antiferromagnetism is expected to settle for smaller Cr thicknesses,[23,20] presumably affecting the $N^{-3/2}$ behavior. Therefore, assuming perfect interfaces, it is not correct, or at least not rigorous, to use asymptotic expressions (derived for noninteracting Cr) to analyze numerical or experimental values of $J(N)$ in Fe/Cr/Fe(001) trilayers for Cr layer thick-

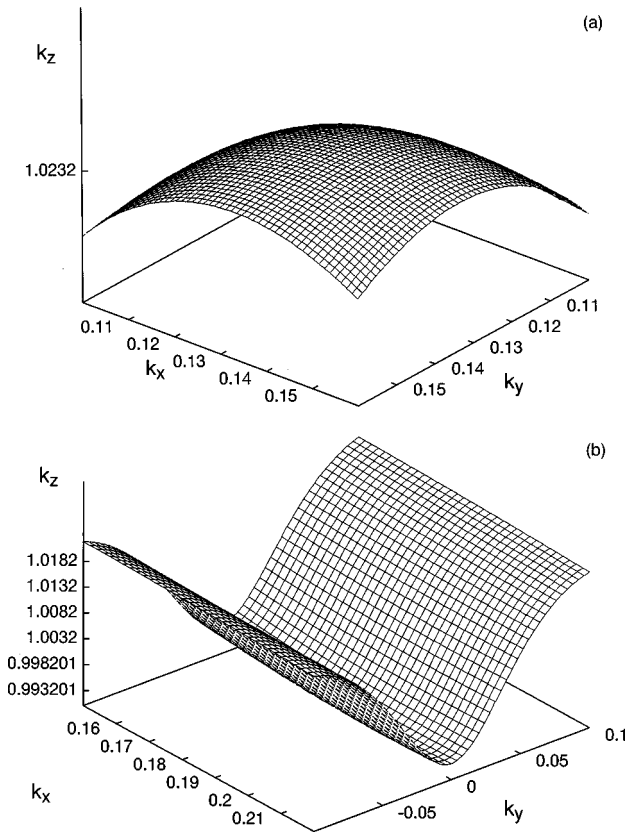

FIG. 4. Nesting of the electron and hole octahedralike Cr FS sheets along the (001) direction (see text), calculated around its extrema, located in the lines $k_x = k_y$ (a) and $k_y = 0$ (b), respectively.

nesses <30 atomic planes. It is also unwise to use them to analyze experimental results for $J(N)$, showing short period oscillations, for $N>30$ atomic planes because for such thicknesses the Cr spacer layer is probably magnetic. The fact that it is possible to find good fits of calculated or experimental results using Eqs. (1) and (2) does not mean that the parameters obtained are necessarily trustworthy. However, in those samples where the short period contributions are suppressed and the long period is prominent, $J(N)$ is no longer expected to decay asymptotically as $N^{-3/2}$ as we have found at $T=0$ K. In this case, it is possible that $J(N,T)$ follows Eq. (1) for sufficiently large values of N because, as mentioned earlier, there are strong indications that the long-period contribution comes from isolated FS singularities. Nevertheless, before using Eq. (1) to analyze the coupling, one must be certain that, in practice, the asymptotic regime has been reached and that a SDW state is not present in the Cr spacer layer for such thicknesses.

We now turn to the temperature dependence of the coupling. We have calculated J_1 for several temperatures and Cr spacer thicknesses. For temperatures between 0 and 500 K, and Cr layer thicknesses varying from 5 to 50 atomic planes, we have found, assuming perfect interfaces, that the coupling is entirely dominated by short-period oscillations. Our results contrast with those of Ref. 42, where it was found that for temperatures $T \geqslant 300$ K the long period oscillation prevails for Cr thicknesses >7 atomic planes. This is very surprising, since their theoretical framework is the same as ours, and the band structures used are only slightly different. Temperature

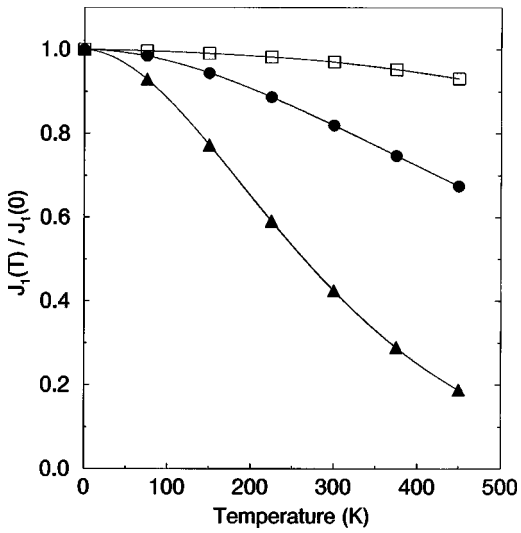

FIG. 5. Temperature dependence of $J_1(N)$ for selected Cr thicknesses: $N=5$ (squares), $N=10$ (full circles), and $N=23$ (triangles).

effects in both calculations come solely from the temperature dependence of the Fermi function. No spin fluctuations in the ferromagnetic layers are taken into account, which is a reasonable approximation for the range of temperatures considered, namely T much smaller than the Fe Curie temperature.

To verify our numerical approach we have thoroughly tested both the energy and Brillouin-zone numerical integrations involved in our calculations of $J(N,T)$. We have performed the energy integration in the complex plane, using Matsubara frequencies at finite temperatures and Gauss-Legendre quadrature at $T=0$ K. For the two-dimensional Brillouin-zone integration we have used the number of special $k_\parallel$ points[43] necessary to ensure a relative precision of 10^{-2} in our final results. The short-period contributions are not suppressed in our calculations for $T=300$ K, and this is supported by the results of Ref. 28, which compare extremely well with ours, particularly for N ranging between 10 and 20 atomic planes. The results of Ref. 28 were obtained for a temperature comparable to 235 K using spin-density-functional theory to calculate the change in total energy between the ferromagnetic and antiferromagnetic configurations of the trilayer.

There is consensus about the fact that, at $T=0$ K, the short-period oscillations dominate the coupling in Fe/Cr/Fe (001) trilayers with perfect interfaces, for all values of N.[19,27,34,44] Estimated ratios between the short- and long-period amplitudes vary from ≈ 5 to 10. In fact, from the heights of the peaks in Fig. 1(b) we obtain a ratio of ≈ 7, for large values of N. Therefore, in order to become imperceptible at $T \geqslant 300$ K for $N>7$, as found in Ref. 42, the short-period contribution would need to decay much faster than the long period one. The temperature dependence of J is governed by geometrical aspects of the spacer Fermi surface and by the confining strength of the magnetic layers. These quantities are determined by the electronic structure of the trilayer, which seems to be reasonably well described in all these calculations. It is unlikely that small differences between the band structures could lead to such a radical change of behavior. Therefore, the reason why our results and those of Ref. 28 differ from Ref. 42 remains a mystery.

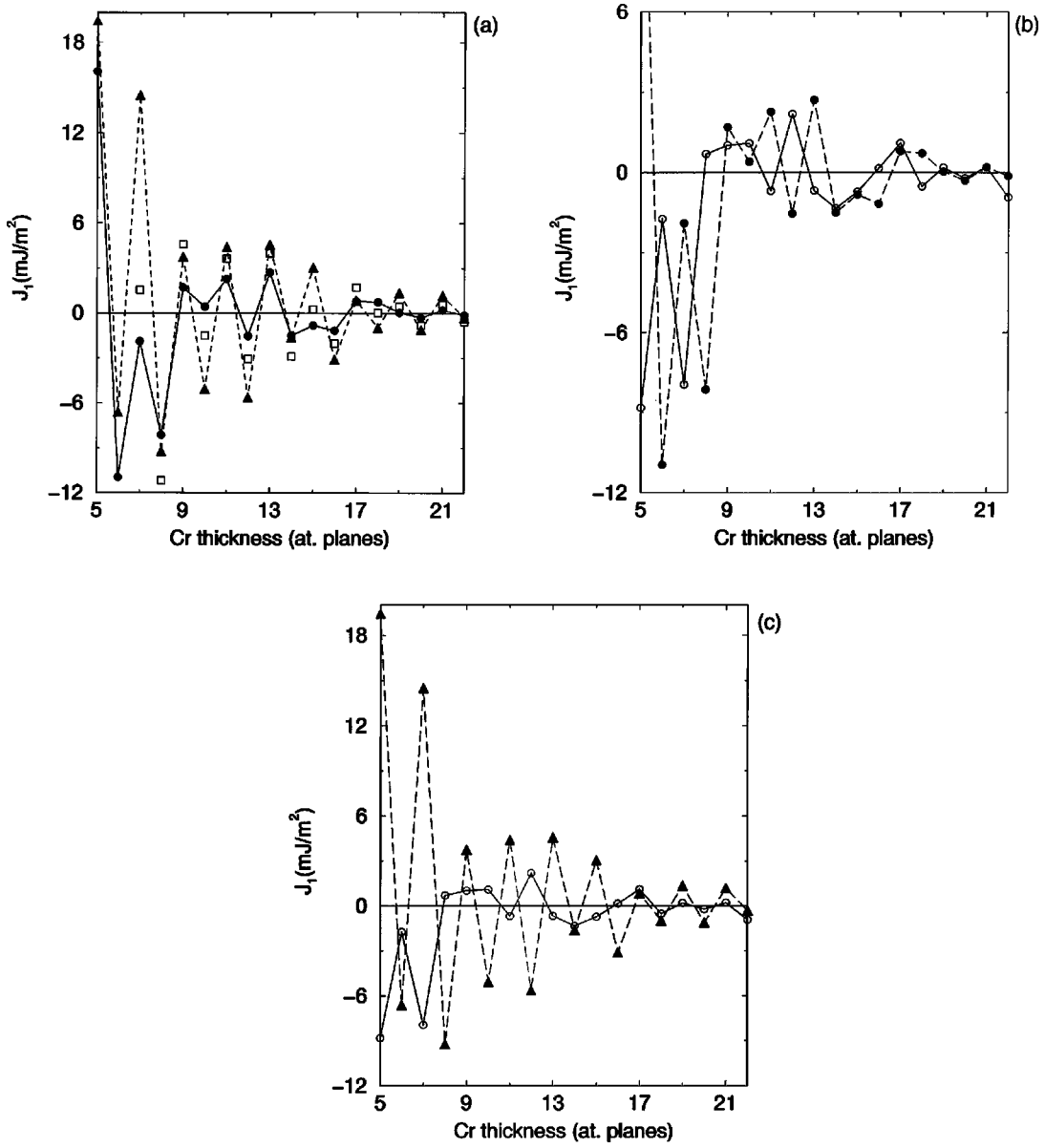

FIG. 6. Calculated exchange coupling considering different interface mixings. Results are obtained at $T=300$ K as a function of the number N of Cr atomic planes. (a) Interface mixing restricted to two atomic planes, comparison between different concentrations: Fe/$Cr_{1-p}Fe_p$/$Fe_{1-p}Cr_p$/Cr/Fe(001) trilayers with $p=1$ (triangles), $p=0.9$ (squares), and $p=0.75$ (filled circles); (b) Interface mixing with different spatial extents: mixing confined to two atomic planes with $p=0.75$ (filled circles), and four atomic planes, i.e., Fe/$Cr_{1-p}Fe_p$/$Cr_{1-q}Fe_q$/$Fe_{1-q}Cr_q$/$Fe_{1-p}Cr_p$/Cr/Fe(001) trilayers, with $p=0.80$ and $q=0.75$ (open circles). (c) Comparison with perfect interfaces corresponding to $p=q=1$ (triangles) and $p=0.80$, $q=0.75$ (open circles).

As shown in Fig. 5, we have obtained a very strong reduction of the coupling as a function of temperature for some values of N. Our results agree very well with experimental observations.[45,46] It should be pointed out, however, that the latter were made on samples showing basically a long period oscillatory $J(N)$. In this case one may argue that it would be reasonable to analyze the experimental data with Eq. (1), since the conditions for using it seem to be at least partially satisfied. It is clear from Eqs. (1) and (2) that when the coupling shows only one periodic component, coming from an isolated singularity of the spacer FS, its temperature dependence can be written, for sufficiently large values of N, as $J(N,T)/J(N,0)=(T/T_0)/\sinh(T/T_0)$, where $T_0^{-1}=k_B(BN+C)$. The same temperature dependence is obtained by Ruderman-Kittel-Kasuya-Yosida and earlier quantum-well theories,[3,6] except for the C term, which has been incorporated later and shown to be very important in Co/Cu systems.[36] In fact, the experimental data obtained in Ref. 46 were very well fitted by this expression even though it was unnecessarily assumed that $C=0$.

III. EFFECT OF INTERFACIAL MIXING

The quality of interfaces in multilayer systems depends on the substrate temperature during layer deposition. Experimentally, it is very difficult to avoid the occurrence of interface inhomogeneities in these systems. As far as the oscillatory coupling between magnetic layers is concerned, we know that variation of interfacial quality alters the degree of carrier confinement in the spacer, causing a phase change

and an overall reduction of the coupling strength. It may also modify the relative contributions of the different periodic components of $J(N)$. In fact, it has been explicitly shown that the amplitude of the short-period oscillations of $J(N)$ in Fe/Cr can be strongly attenuated by interfacial roughness.[18]

The temperature of optimal (layer-by-layer) growth varies from system to system, and for Fe/Cr(001) multilayers it is $T=300\,^{\circ}\mathrm{C}$. Nevertheless, even under optimal conditions, the Cr growth on Fe(001) leads to formation of a Cr-Fe alloy in approximately three interfacial atomic planes.[21] The alloying is an asymmetric effect which happens only when Cr is deposited on Fe but not vice versa. According to scanning tunneling studies, for the $300\,^{\circ}\mathrm{C}$ growth condition, the Cr concentration in Fe seems not to exceed 10%. However, Auger spectroscopy estimates that it can be as much as 40%.[29]

It is reasonable to attribute the large difference between calculated and measured values of the coupling in Fe/Cr systems to the probable existence of inhomogeneities in the samples. However, one must quantitatively verify their effect in the calculated results. With this purpose, we have investigated the effect of mixing at the Fe/Cr interface by treating the interfacial Fe/Cr atomic planes as disordered alloys compatible with a given concentration profile. We restrict ourselves to moderate interfacial admixtures, and assume that it takes place at either two or four atomic planes of the Fe/Cr interface. The effect of disorder is treated within the average *t*-matrix approximation which, in the dilute limit, is equivalent to the coherent-potential approximation used in Refs. 47 and 48. Our results are presented in Fig. 6. First, we calculate the coupling as a function of the Cr spacer thickness assuming that the interface mixing is confined to two atomic planes, considering Fe/Cr alloys with different concentrations at the interface. More specifically, in Fig. 6(a) we examine $\mathrm{Fe/Cr}_{1-p}\mathrm{Fe}_p/\mathrm{Fe}_{1-p}\mathrm{Cr}_p/\mathrm{Cr/Fe(001)}$ trilayers, with $p=1.0$, 0.9, and 0.75. It is evident that the overall amplitude of the coupling decreases, and the short-period oscillations tend to be progressively washed out with increasing interfacial mixing. However, the reduction in the coupling amplitude in Fe/Cr is not so dramatic as found in Co/Cu multilayers.[48] In Fig. 6(b) we investigate the effect of broadening the region in which the interface mixing occurs. We compare results of the previous calculation corresponding to $p=0.75$ with the case in which the mixing is confined to four atomic planes, more precisely with $\mathrm{Fe/Cr}_{1-p}\mathrm{Fe}_p/\mathrm{Cr}_{1-q}\mathrm{Fe}_q/\mathrm{Fe}_{1-q}\mathrm{Cr}_q/\mathrm{Fe}_{1-p}\mathrm{Cr}_p/\mathrm{Cr/Fe}$ (001) trilayers, with $p=0.80$ and $q=0.75$. We note that upon increase of the spatial extent of the interface mixing, the overall amplitude of the coupling decreases further, and a phase shift in the oscillations becomes apparent. This is expected because, as mentioned earlier, both the amplitudes and phases of the oscillatory components of the interlayer coupling depend on the degree of carrier confinement in the spacer caused by the magnetic layers, which is obviously affected by interface mixing. Finally, to assess the overall effect of interface mixing we compare in Fig. 6(c) the latter results corresponding to $p=0.80$ and $q=0.75$ with those for perfect interfaces. It is clear that the short-period oscillations are substantially suppressed by interface mixing. However, the calculated coupling amplitude is effectively reduced only by approximately a factor of 3 for the maximum amount of interface mixing which we have considered. This is still not sufficient to establish reasonable agreement with experimental data. One possibility to close such a gap would be to assume larger amounts of interface mixing. However, one should note that the presence of steps, which has been ignored in our calculations, but are probably present in real samples, also contributes to diminish the interlayer coupling amplitude, and its short-period oscillatory components.[48,49] If the steps are sufficiently large it is possible to assess their effect by taking averages of the coupling calculated for different spacer thicknesses. A rough estimate, assuming thickness fluctuations of ± 1 atomic plane, can be obtained by taking a simple average $\langle J(N)\rangle=[J(N-1)+2J(N)+J(N+1)]/4$, as depicted in Fig. 7. We notice that the presence of steps at the Fe/Cr interface, combined with interface mixing, practically removes the residual short-period oscillations, reducing the coupling amplitude even further, in agreement with what has been found in Ref. 18. Nevertheless, the calculated value at the first AF peak remains a factor of five larger than those measured.

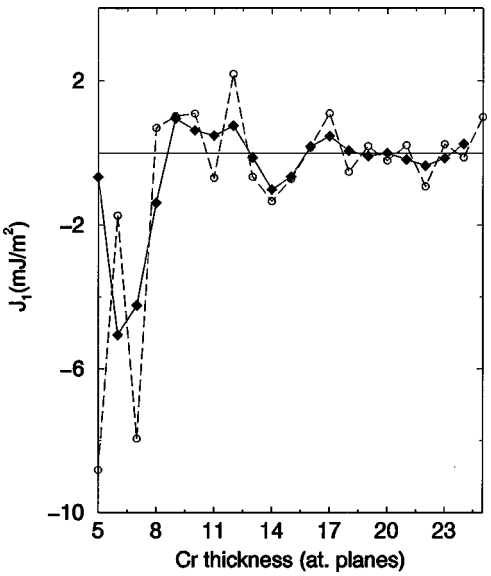

FIG. 7. Comparison between the values of $J_1(N)$, calculated at $T=300$ K for $\mathrm{Fe/Cr}_{1-p}\mathrm{Fe}_p/\mathrm{Cr}_{1-q}\mathrm{Fe}_q/\mathrm{Fe}_{1-q}\mathrm{Cr}_q/\mathrm{Fe}_{1-p}\mathrm{Cr}_p/\mathrm{Cr/Fe}$ (001) trilayers, with $p=0.80$ and $q=0.75$ (open circles), as a function of N, and the corresponding average values obtained by $\langle J_1(N)\rangle=[J_1(N-1)+2J_1(N)+J_1(N+1)]/4$ (filled diamonds). These results give an idea of the combined effect of interface mixing and the presence of steps at the Fe/Cr interface.

IV. CONCLUSIONS

We have calculated the coupling between Fe layers separated by noninteracting Cr in Fe/Cr/Fe(001) trilayers as a function of the Cr layer thickness for several temperatures. We have found that for perfectly sharp interfaces the short-period oscillations are the dominant contributions to $J(N,T)$ for $0\leqslant T\leqslant 500$ K and $1\leqslant N\leqslant 30$ atomic planes. We have also shown that at zero temperature the amplitude of $J(N)$ decays as $N^{-3/2}$ for large values of N, rather than as N^{-2} or N^{-1} as usually assumed. This behavior is caused by the particular type of singularity in the nesting of the Cr FS (along the lines $k_y=0$ and $k_x=0$) which is responsible for one of the dominant short-period oscillatory contributions to $J(N)$.

It must be pointed out, however, that the $N^{-3/2}$ asymptotic decay, predicted for noninteracting Cr, happens for such large values of N that, in practice, the Cr layer would develop a SDW antiferromagnetism which presumably affects this type of behavior. Our results obtained at finite temperatures show a strong temperature dependence of the coupling strength for some values of the Cr spacer thickness, in very good agreement with experiments.

All existing calculations, including ours, for Fe/Cr/Fe (001) trilayers with perfect interfaces have found interlayer coupling strengths which are at least an order of magnitude larger than those experimentally observed at the first AF peaks. On the other hand, it is currently very difficult, if not impossible, to avoid the appearance of inhomogeneities in Fe/Cr interfaces. The absence of strong short-period oscillatory components, and the existence of a relatively large biquadratic contribution in the measured coupling are strong evidence of the presence of inhomogeneities in the sample. We have assessed the reduction of the coupling amplitude due to their presence at the interfaces. We have found that interface mixing reduces the overall coupling strength, as well as the relative importance of its short-period oscillatory components, and also causes a phase shift in the oscillations of the interlayer coupling. However, our results indicate that moderate interface mixing alone does not seem to be sufficient to bring theory in accord with experiment. The combined effect of the presence of steps and moderate mixings at the Fe/Cr interface leads to better, but still far from perfect agreement. Therefore, either there is something important missing in all existing calculations or currently the samples have far more inhomogeneities than they seem to. We stress that our results are for trilayers and, therefore, apply to multilayers with sufficiently thick Fe layers only.

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