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Reflection-amplitude Approximation for the Interlayer Exchange Coupling in (001) Co/Cu/Co Multilayers

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Abstract

The reflection-amplitude approximation is used to calculate the interlayer exchange coupling in (001) Co/Cu/Co multilayers. The dependence of the phase factor of the reflection amplitude on the energy and wave vector is included. The contribution of each period is calculated and the results are compared with those from the asymptotic behavior. It is shown that the energy and wave-vector dependence of the phase factor may affect the interlayer exchange coupling significantly.

1. Introduction

Since the discovery of the antiferromagnetic coupling between two adjacent Fe layers separated by Cr layer [1], the interlayer exchange coupling has drawn much interest. The underlying mechanism for the interlayer exchange coupling in magnetic multilayers has been attributed to the spin-dependent quantum interference in the spacer [2-4]. Among the many theoretical approaches, a simple model associated with the reflection amplitude is very useful for its physical transparency [3,4]. This reflection-amplitude approximation has been successfully applied to explain the origin of multiple periods of the interlayer exchange coupling in magnetic multilayers [5-7]. Recently, we modified this model by including the dependence of the argument of the reflection amplitude on the energy and wave vector and better agreement was obtained between the approximation and the full-band calculation for (111) Co/Cu/Co trilayer [8]. In this paper, we apply the modified reflection-amplitude approximation to (001) Co/Cu/Co and calculate contribution of each period to the interlayer exchange coupling.

2. Theoretical Model

In this section, we briefly review the derivation of the reflection-amplitude approximation for the interlayer exchange coupling. Details can be found in Ref. [8]. The interlayer exchange coupling is defined as

$$J = \frac{\Omega_F - \Omega_{AF}}{2S}, \tag{1}$$

where Ω_F and Ω_{AF} are the grand canonical potentials for the ferromagnetic (F) and antiferromagnetic (AF) configurations and S is the area of the sample. The difference in the grand canonical potential between the bulk and the multilayer systems is given by the force theorem as

$$\Delta\Omega^{\nu} = \frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}_{\parallel}}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\,\mathrm{Tr}\ln(1 - G_0 T^{L,\nu} G_0 T^{R,\nu}), \tag{2}$$

where ν labels the two configurations (F and AF), G_0 is the bulk Green's function, T is the T-matrix, f is the Fermi-Dirac distribution, and L and R stand for the left and right interface, respectively. Tr denotes the trace including the spin index and $\mathbf{k}_{\parallel}$ is the wave vector parallel to the plane. The T-matrix can be replaced by the reflection amplitude at the interface and only the first order term is kept in the logarithm such as

$$\ln(1 - G_0 T^L G_0 T^R) = \ln(1 - r_L r_R e^{iqD}) \approx -r_L r_R e^{iqD}, \tag{3}$$

where r_L (r_R) is the reflection amplitude from the left (right) interface and D is the thickness of the spacer. The growth direction is taken as z-axis, and the spanning vector q is $q = k_i - k_r$, where k_i and k_r are z-components of the incident and reflected wave vector, respectively. When the energy integral is performed with complex residue theory, the exchange coupling is

$$J = \frac{k_B T}{\pi^2}\mathrm{Re}\sum_{n=0}^{\infty}|\Delta r|^2 e^{i(qD+2\phi_r)}\Big|_{\varepsilon=\varepsilon_F + i(2n+1)\pi k_B T}, \tag{4}$$

where $\Delta r = (r^+ - r^-)/2$ is the spin-asymmetry of the reflection amplitude with reflection amplitude r^+ (r^-) for the majority (minority) spin and ϕ_r

is the argument of Δr ($\Delta r = |\Delta r| e^{i\phi_r}$). For the summation over Matsubara frequencies, the phase factor is approximated by

$$qD + 2\phi_r \approx q_F D + 2\phi_{rF} + \left(\frac{\partial q}{\partial \varepsilon} + 2\frac{\partial \phi_r}{\partial \varepsilon} \right)(\varepsilon - \varepsilon_F), \tag{5}$$

where q_F is the spanning vector which connects the Fermi surface for a given $\mathbf{k}_{\parallel}$. After the summation, the interlayer exchange coupling is

$$J = \frac{2k_B T}{\pi^2} \mathrm{Re} \frac{|\Delta r_F|^2 \, e^{i(q_F D + 2\phi_{rF})}}{\sinh[2\pi k_B T (D/\hbar v_F + \partial\phi_r/\partial\varepsilon)]}, \tag{6}$$

where v_F is the magnitude of the group velocity at the Fermi level. The integration over $\mathbf{k}_{\parallel}$ is done by using the stationary phase approximation. In general the stationary point is given by

$$\nabla_{\mathbf{k}_{\parallel}} (q_F D + 2\phi_{rF}) = 0, \tag{7}$$

which is not necessarily the extremal point of the Fermi surface. However, we will consider only the case of $\nabla_{\mathbf{k}_{\parallel}}(q_F) = 0$ and $\nabla_{\mathbf{k}_{\parallel}}(\phi_{rF}) = 0$ at the extremal point and also assume that q_F and ϕ_{rF} have the same principal axes, k_x and k_y. We expand $q_F D + 2\phi_{rF}$ as a function of $\mathbf{k}_{\parallel}$ such as,

$$q_F D + 2\phi_{rF} \approx q_F^0 D + 2\phi_{rF}^0 + \frac{D + D_x}{\kappa_x}(k_x - k_x^0)^2 + \frac{D + D_y}{\kappa_y}(k_y - k_y^0)^2, \tag{8}$$

where κ_x and κ_y are determined by the curvature of the Fermi surface with $2/\kappa_x = \partial^2 q_F / \partial k_x^2$ and $2/\kappa_y = \partial^2 q_F / \partial k_y^2$ and D_x and D_y are

$$D_x = \kappa_x \frac{\partial^2 \phi_{rF}}{\partial k_x^2} \tag{9}$$

and

$$D_y = \kappa_y \frac{\partial^2 \phi_{rF}}{\partial k_y^2}. \tag{10}$$

The derivatives are calculated at the extremal point. By using the stationary phase approximation, the interlayer exchange coupling is

$$J = \mathrm{Im}\frac{\hbar v_F \kappa n}{4\pi^2}\frac{|\Delta r_F|^2\, e^{i(q_F^0 D + 2\phi_{rF}^0 + \phi)}}{(D+D_\varepsilon)\sqrt{|(D+D_x)(D+D_y)|}} F[(2\pi k_B T/\hbar v_F)(D+D_\varepsilon)], \quad (11)$$

where $\kappa = \sqrt{|\kappa_x \kappa_y|}$, n is the number of the same kind of extremal points, and $F(x) = x/\sinh(x)$. The additional phase factor ϕ is $\phi = 0, \pi/2, \pi$ when $(D+D_x)/\kappa_x$ and $(D+D_y)/\kappa_y$ have both positive, different, and both negative signs, respectively. D_ε is given by $D_\varepsilon = \hbar v_F\, \partial\phi_r/\partial\varepsilon$. When D_ε, D_x, and D_y are ignored, the interlayer exchange coupling becomes the well-known asymptotic form

$$J = \mathrm{Im}\frac{\hbar v_F \kappa n}{4\pi^2 D^2}(\Delta r)^2 e^{i(q_F^0 D + \phi)} F(2\pi k_B T D/\hbar v_F). \quad (12)$$

3. (001) Co/Cu/Co Trilayer

There are two kinds of extremal points for (001) Co/Cu/Co. The long period is from the extremal spanning vector at the belly of the Fermi surface and the short period corresponds to the neck. An sp^3d^5 tight-binding model is adopted for the band structures of Cu and Co [5]. The reflection amplitude is calculated with Co/Cu interface. In general, the reflection amplitude is a complex number for realistic band structures. As shown in Eqs. (4) and (6), not only $q_F D$ but also ϕ_r contributes to the phase factor of the exponential function and it should be included unless the spacer is very thick or ϕ_r is constant.

In Fig. 1, the phase factor ϕ_r of the reflection amplitude is plotted as a function of energy at the extremal point. The solid line is for the long period [$\mathbf{k}_\parallel = (0,0)(2\pi/a)$] and the dotted line is for the short period [$\mathbf{k}_\parallel = (0.41,0.41)(2\pi/a)$], where a is the lattice constant of Cu. The Fermi energy is $\varepsilon_F = 0$. The phase factor ϕ_r changes significantly as a function of the energy and it cannot be ignored for the short period [see Eq. (5)]

unless D is very big. We plot the phase factors as functions of the wave vector in Figs. 2 and 3 for the long and the short period, respectively. For the both periods, ϕ_r varies much as $\mathbf{k}_{\|}$ does. For the long period, the dependence of ϕ_r on the other principal axis k_{010} is the same as Fig. 2 due to the symmetry. The principal axes for the short period are taken as k_{110} and $k_{1\bar{1}0}$. In Fig. 3, the phase factor ϕ_r is plotted along k_{110}. Along this direction, the point of $\nabla_{\mathbf{k}_{\|}}(\phi_{rF})=0$ does not exactly coincide with that of $\nabla_{\mathbf{k}_{\|}}(q_F)=0$. This can happen for the extremal point with lower symmetry. However, in the case of the short period of (001) Co/Cu/Co, the difference is very small [$\Delta k_{110} \approx 0.005(2\pi/a)$] and ignored.

The long period and short period contributions to the interlayer exchange coupling of (001) Co/Cu/Co as a function of the spacer thickness D are given in Figs. 4 and 5, respectively. The temperature is taken as T=300 K. The interlayer exchange coupling can be obtained by adding these two contributions. The solid curve is from the reflection-amplitude approximation of Eq. (11) and the dotted curve is from the asymptotic from of Eq. (12). In Fig. 4, the parameters due to the phase factor ϕ_r are $D_\varepsilon \approx -2.7$ monolayers (ML) and $D_x = D_y \approx 16$ ML. Compared to the dotted curve, the overall coupling strength is reduced because of D_x and D_y. But, the coupling becomes much stronger near $D=3$ ML due to D_ε. For the short period, the parameters are calculated as $D_\varepsilon \approx 17$ ML, $D_x \approx 8.2$ ML, and $D_y \approx -13$ in Fig. 5. The singular behavior near $D=13$ ML is due to the negative D_y and the failure of the stationary phase approximation [8]. The interlayer coupling of such cases should be obtained from the full-band calculation. By comparing the solid and the dotted curve, it can be seen that the phase factor changes the interlayer coupling more significantly for the short period. The coupling strength for the thin spacers is much reduced due to the phase factor. Although the accurate coupling strength for the thin spacers can be obtained only by the full-band calculation, the coupling strength for the short period of this work is comparable to the experimentally measured one $J \approx 0.4\,\mathrm{mJ/m^2}$ [9]. Note that the experimentally measured coupling strengths are smaller than the theoretical ones because of the roughness at the interface of the sample. For the short period, D_ε is rather big and affects the temperature dependence of the interlayer exchange coupling as can be seen in Eq. (11).

4. Conclusion

The interlayer exchange coupling of (001) Co/Cu/Co is calculated from the reflection-amplitude approximation. The long period and the short period contributions are considered separately. The dependence of the phase factor of the reflection amplitude affects the interlayer coupling significantly and cannot be ignored for the both periods. The interlayer coupling of (001) Co/Cu/Co is dominated by the short period. The coupling strength for the short period decreases much when the dependence of the phase factor is included in the reflection-amplitude approximation.

Acknowledgements

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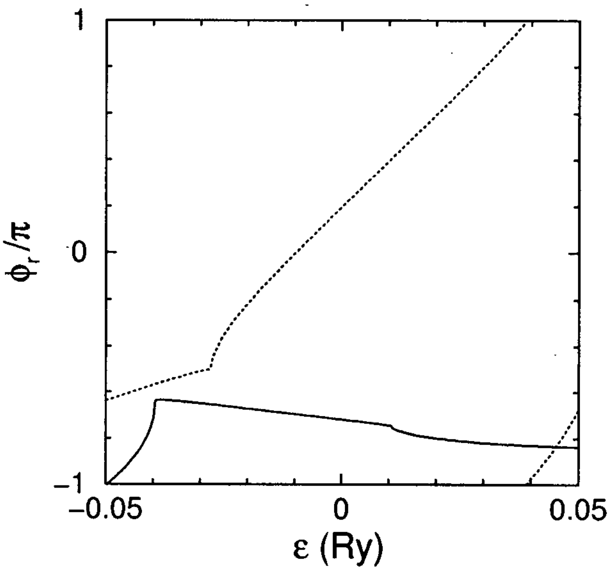

Fig. 1. The argument ϕ_r of the reflection amplitude as a function of energy at the extremal point. The solid line is for the long period and the dotted line is for the short period.

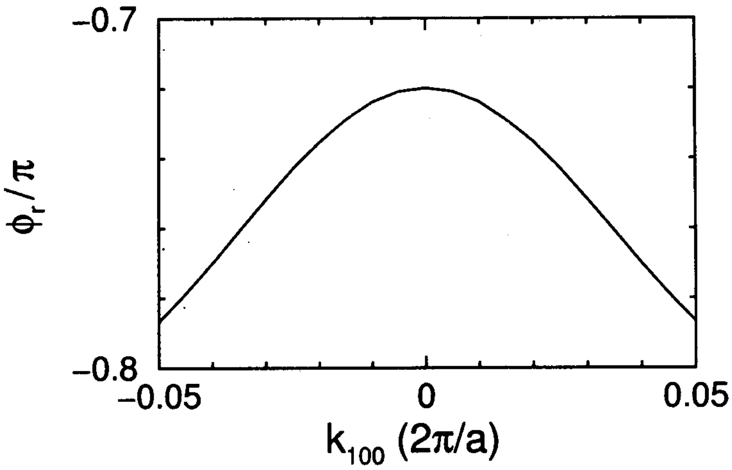

Fig. 2. The phase factor of the reflection amplitude as a function of the wave vector near the stationary point for the long period of (001) Co/Cu/Co.

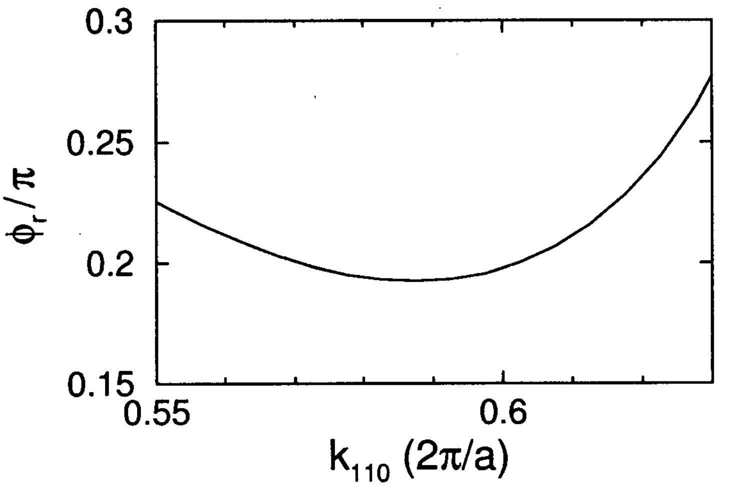

Fig. 3. The phase factor of the reflection amplitude as a function of the wave vector near the stationary point for the short period of (001) Co/Cu/Co.

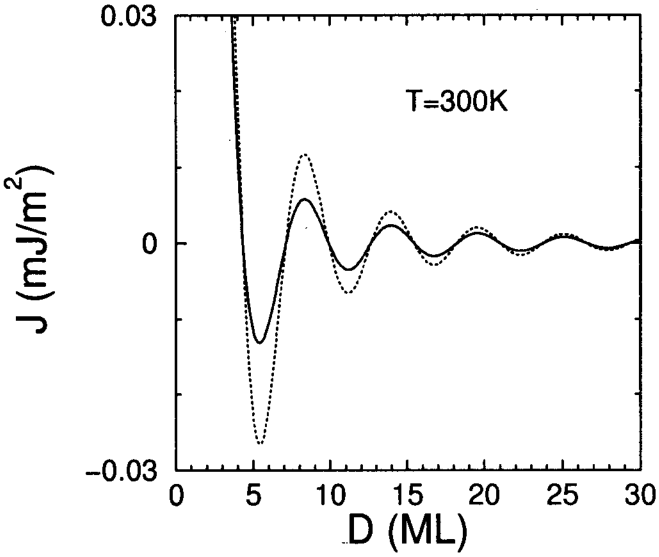

Fig. 4. Long period contribution to the interlayer exchange coupling of (001)Co/Cu/Co as a function of the spacer thickness D at the temperature T =300 K. The solid curve is from the reflection-amplitude approximation and the dotted curve is from the asymptotic from.

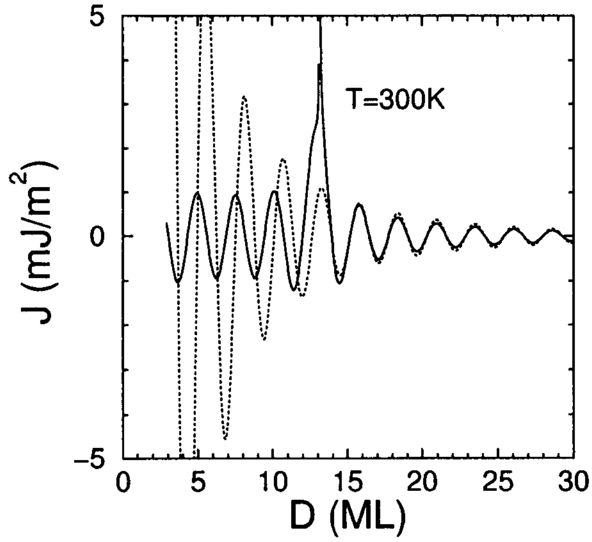

Fig. 5. Short period contribution to the interlayer exchange coupling of (001)Co/Cu/Co as a function of the spacer thickness D at the temperature T =300 K. The solid curve is from the reflection-amplitude approximation and the dotted curve is from the asymptotic from.