PHYSICAL REVIEW B VOLUME 57, NUMBER 9 1 MARCH 1998-I

Magnetic-sublayers effect on the exchange-coupling oscillations versus cap-layer thickness

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(Received 24 July 1997; revised manuscript received 29 October 1997)

We have found that some periods of interlayer-exchange-coupling (IEC) oscillations as a function of cap-layer (CL) thickness may be suppressed if the in-plane extremal spanning vectors of the cap- and ferromagnet-material Fermi surfaces do not coincide. The suppression of the IEC oscillations versus the CL thickness holds also if the magnetic slab thickness tends to infinity. On the one hand, we have shown by means of very simple arguments that apart from the well-known selection rules concerning the spacer and cap layers another rule related to the magnetic sublayers has to be fulfilled for the interlayer coupling oscillations versus CL thickness to survive. On the other hand, the distribution of induced magnetic moments across the nonmagnetic cap and spacer sublayers has been computed and shown to reveal the underlying periodicity of the materials they are made of (i.e., related to their bulk Fermi surfaces) independently of whether or not the selection rules are fulfilled. This means that the IEC oscillations are of global nature and depend on all the sublayers that constitute the system. [S0163-1829(98)06709-5]

I. INTRODUCTION

Magnetic multilayers have been intensively studied for over a decade now.[1–3] The reasons are, apart from challenging cognitive aspects, (already partially realized) practical applications of superlattices as magnetoresistive sensors, angular velocity meters, recording heads, and magnetic memory elements. The phenomenon most of these applications is based on is the well-known giant magnetoresistance (GMR) coming from a strong electron-spin dependence of resistivity in magnetic systems. To optimize devices of that sort, it is necessary to test the effect of all of the ingredients of the system in question (including kind of materials they are made from and thicknesses of particular sublayers) either directly on GMR or indirectly on the interlayer exchange coupling (IEC). Obviously, the effect of a spacer on IEC was established first[3,4] and then that due to magnetic sublayers;[5–10] finally the cap-layer (CL) effect has been studied quite recently.[11–15]

Before we present our original results let us briefly recall the most important facts concerning the CL's: (i) The IEC oscillates as a function of CL thickness with a period determined by extremal $\vec{k}$ spanning vectors of the CL Fermi surface, (ii) a bias of the oscillations (their asymptotic value) depends on spacer thickness,[11,14,15] (iii) the IEC oscillations are strongly suppressed if stationary in-plane spanning vectors of the CL Fermi surface do not coincide with their counterparts of the spacer Fermi surface,[14,15] and (iv) the direct and inverse photoemissions[16,17] on various combinations of overlayers deposited on different films show a periodic distribution of the so-called quantum-well states (QWS's) with periods determined by extremal spanning vectors of the overlayer Fermi surface. We shall refer to the latter only indirectly, by exploiting the fact that the QWS's lead to some spin polarization of nonmagnetic cap layers.

The aim of the present paper is to emphasize the relevance of magnetic sublayers to IEC oscillations as a function of CL thickness. In addition, we shall comment on induced magnetic moments in the nonmagnetic sublayers, which may be viewed as a manifestation of the quantum-well states.[16–19]

II. METHOD

Our earlier papers[6,20,21] based on the single-band tight-binding model have proved that the model we use gives a reasonable qualitative description of basic physical mechanisms responsible for oscillatory phenomena in magnetic trilayers. Our Hamiltonian, described in detail in Ref. 21, consists of the nearest-neighbor hopping and spin-dependent on-site potential terms. The systems under consideration now are trilayers capped with an overlayer, of the type $n_{ovr}O/n_fF/n_sS/n_fF$, where n_{ovr}, n_f, and n_s stand for the numbers of cap (O), ferromagnetic (F), and spacer (S) monolayers in the perpendicular z direction. Hereinafter the subscripts and superscripts ovr and s will always refer to the cap and spacer layers, whereas the spin-dependent parameters referring to ferromagnetic sublayers will be indexed by $\sigma=\uparrow$ or $\downarrow$. For simplicity, we restrict ourselves to a simple cubic structure and regard the lattice constant and the hopping integral as the length and energy units, respectively.

The interlayer exchange coupling has been calculated from the difference in thermodynamic potentials exactly as in Ref. 21. Moreover, the magnetic moments (including the induced ones) m have been expressed in terms of the eigenfunctions u of the Hamiltonian as $m_i=n_{i\uparrow}-n_{i\downarrow}$, with $n_{i\sigma}=\Sigma_E|u_{i,\sigma}(E)|^2$, where the summation runs over occupied states.

III. ASYMPTOTIC LIMITS

In this section we present some analytic formulas that will be useful for the interpretation of rigorous numerical results of Sec. IV. As has been shown in Ref. 22, the IEC can be Fourier transformed with respect to n_s and n_σ. That procedure can be quite straightforwardly generalized to include the CL thickness as well. The resulting asymptotic (within the stationary phase approximation) expression consists of the terms of the form $A_{pqrn}(\vec{k}_\parallel,E_F)\exp\{2i[pk_z^s n_s+(qk_z^\uparrow+rk_z^\downarrow)n_f+nk_z^{ovr}n_{ovr}]\}$ summed over all the in-plane wave vectors for which the exponential is stationary. The A coefficients are defined analogously to those in Ref. 22. Their exact numerical values are not important for qualitative considerations; we note only that all the amplitudes of oscillations vanish asymptotically with the given sublayer thickness going to infinity.[22] There exist, however, some additional restrictions imposed by the asymptotic behavior of the IEC. In particular, a direct generalization of the results of Ref. 22 to the present case, with the cap layer, gives $A_{0qrn}=0$ (no coupling for $n_s\to\infty$). Another limit to be taken is $n_f\to\infty$, when, in view of the above-mentioned asymptotic behavior, all the terms tend to zero except for A_{p000} and A_{p00n}. Since the oscillations versus spacer thickness survive in this limit in contrast to the ones versus the CL thickness that decay (see below), we conclude that $A_{p000}\neq 0$ and $A_{p00n}=0$.

Finally, taking into account the above-mentioned restrictions and keeping for simplicity only the lowest-order harmonics, we arrive at the formula

$$J=\sum_\alpha A_{1000}e^{2ik_z^s n_s}+\sum_{\alpha_1} A_{1100}e^{2i(k_z^s n_s+k^\uparrow n_f)}+\sum_{\alpha_2} A_{1010}e^{2i(k_z^s n_s+k_z^\downarrow n_f)}+\sum_{\alpha_3} A_{1101}e^{2i(k_z^s n_s+k_z^\uparrow n_f+k_z^{ovr}n_{ovr})}+\sum_{\alpha_4} A_{1011}e^{2i(k_z^s n_s+k_z^\downarrow n_f+k_z^{ovr}n_{ovr})}+\cdots, \tag{1}$$

where the α's are the sets of in-plane wave vectors for which the relevant exponentials are stationary. For the case of the CL thickness dependence this allows us to formulate the present selection rule, which in its general form (for n_s and n_f large and fixed and n_{ovr} large and varying) reads

$$\nabla k_z^{ovr}=0,\quad p\nabla k_z^s n_s+(q\nabla k_z^\uparrow+r\nabla k_z^\downarrow)n_f=0, \tag{2}$$

with nonvanishing p and either q or r (∇ is the two-dimensional gradient in k_x-k_y space). This means that out of all the stationary vectors of the cap material Fermi surface (FS) only those that simultaneously satisfy the above-mentioned conditions for the in-plane gradients give rise to the oscillations with CL thickness. Equation (2) is the main result of the present paper. This condition becomes even simpler in the particular case of the single-band simple cubic model considered hereinafter, when the second part of Eq. (2) separates and all the individual in-plane gradients must vanish (cf. Ref. 22).

The origin of the present selection rule becomes clear if we qualitatively interpret Eq. (1) in terms of the quantum interference model.[23] The first term corresponds to the states reflected once at each of the spacer-ferromagnet interfaces, the second and third terms to the states penetrating one of the magnetic layers and reflected back at the cap-ferromagnet interface, and the last two terms describe states reaching the outer boundary of the cap layer (''vacuum''). It is quite clear therefore that the n_f-dependent phase factor also must be taken into account while performing the stationary-phase approximation.

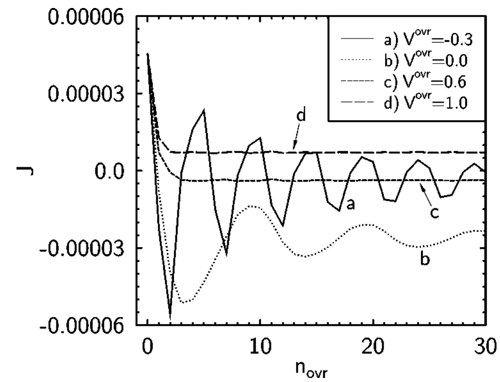

FIG. 1. Exchange coupling vs cap-layer thickness for $n_s=5$, $n_f=3$, $E_F=2.1$, $V^s=V^\downarrow=0$, and $V^\uparrow=-2.0$. Stationary in-plane spanning vectors of the spacer and both the ferromagnetic FS's are $k_\parallel=(\pm\pi,\pm\pi)$. For curves a and b the stationary in-plane vector of the cap FS remains the same, opposite to curves c and d, for which $k_\parallel=(0,\pm\pi),(\pm\pi,0)$ which results in suppressing the oscillations.

It is evident from formula (1) that the bias of oscillations with CL thickness depends not only on the spacer- and magnetic-layer thicknesses but on the on-site V^{ovr} potential as well. The latter observation results from the fact that the A coefficients in the second and third terms of Eq. (1) depend on the value of the reflection coefficient at the cap-ferromagnet interface, which in turn depends on the cap material electronic structure.

The stationary spanning vectors, for a sublayer characterized by the potential V, can be determined in a very simple way by minimizing with respect to $\vec{k}_\parallel$ the following Fermi surface equation for the sc lattice:

$$k_z(\vec{k}_\parallel,E_F)=\arccos[(V-E_F)/2-\cos k_x-\cos k_y]. \tag{3}$$

Hence the in-plane extremal spanning vectors are $\vec{k}_\parallel=(0,0)$ for $-6<E_F-V<-2$, $(\pm\pi,0)$ and $(0,\pm\pi)$ for $-2<E_F-V<2$, $(\pm\pi,\pm\pi)$ for $2<E_F-V<6$, and

$$k_z=\arccos[(V-E_f)/2-\alpha], \tag{4}$$

with $\alpha=2$, 0, and -2 for the corresponding $\vec{k}_\parallel$, respectively. Thus the period of oscillations versus the sublayer (with the potential V) thickness is just $\Lambda=\pi/k_z$ [or $\pi/(\pi-k_z)$].

IV. NUMERICAL RESULTS

We shall now present our exact numerical results (see Ref. 21 for details of the method) and show how they can be interpreted in terms of the analytical formulas from the preceding section. Figure 1 confirms the well-known fact that the IEC oscillations versus CL thickness have a period determined by the kind of material the cap is made of and get suppressed if there is a mismatch in the corresponding in-plane spanning vectors of the CL and the spacer. The suppression takes place in cases c and d, where $\vec{k}_\parallel{}^s=\vec{k}_\parallel{}^\sigma=(\pm\pi,\pm\pi)$, opposite to $\vec{k}_\parallel{}^{over}=(0,\pm\pi),(\pm\pi,0)$. The dependence of the bias values on V^{ovr} is also clearly visible. The magnetic-sublayers effect is presented in Fig. 2, which shows that the suppression may be due to the misfit in the $\vec{k}_\parallel$'s corresponding to the overlayer and magnetic sublayers,

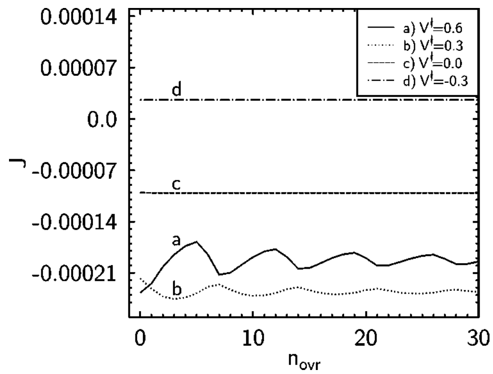

FIG. 2. IEC vs CL thickness for $n_s=5$, $n_f=10$, $E_F=2.1$, $V^s=V^{ovr}=0.3$, and $V^{\uparrow}=-2.0$. Stationary in-plane spanning vectors for the spacer and the cap layer are $k_{\|}=(0,\pm\pi),(\pm\pi,0)$. For curves a and b the minority spin FS stationary points coincide with those of the spacer and the overlayer. For curves c and d both the majority and minority spin Fermi surfaces have the $k_{\|}=(\pm\pi,\pm\pi)$ spanning vector and consequently the IEC oscillations are suppressed.

respectively (curves c and d), whereas for curves a and b the periodicity is quite pronounced owing to the matching of the above-mentioned spanning vectors. It can be also readily seen from Fig. 2 that the phases of oscillations as well as the bias values depend on the potentials of the ferromagnetic layers (exchange splitting). It is noteworthy that Figs. 1 and 2 show that the selection rule works quite well, even when the relevant layer thicknesses are rather small: $n_s=5$ and $n_f=10$, respectively. This confirms our previous observation[21] that relatively small systems in the z direction may reveal the asymptotic behavior. A detailed inspection of curves c and d suggests that the selection rule is slightly more rigorously enforced in Fig. 2 (due to $n_f=10$) than in Fig. 1 (due to $n_s=5$), but the effect is tiny indeed and hardly visible. Incidentally, all the periods of oscillations obtained by the numerical computations and visualized in Figs. 1–4 can be pretty well reproduced in terms of the asymptotic equations (3) and (4); e.g., for $E_F=2.1$ and $V=-0.6$, -0.3, 0.0, 0.3, and 0.6, we get $\Lambda=3.6$, 4.9, 9.9, 6.9 , and 4.3 ML, respectively.

Another rather obvious but noteworthy effect consists in the disappearance of the IEC oscillations versus CL thickness when the magnetic sublayer thickness gets bigger and

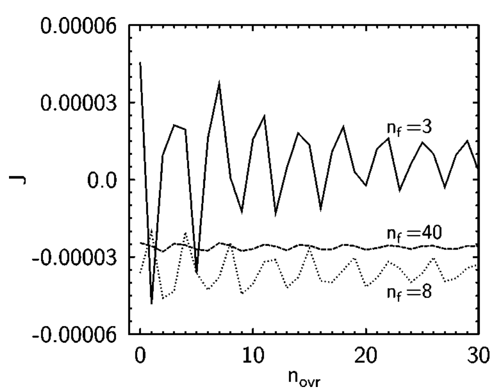

FIG. 3. Effect of magnetic sublayer thickness on the IEC oscillations as a function of cap-layer thickness (the parameters are the same as in Fig. 1 except for $V^{ovr}=-0.6$).

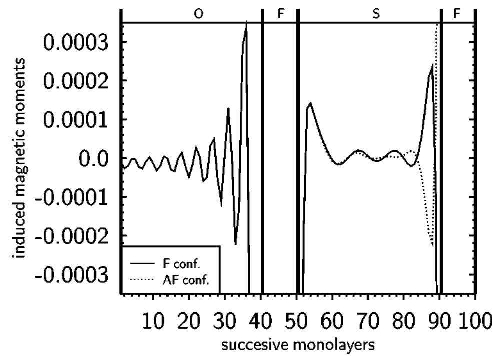

FIG. 4. Induced magnetic moments (with $\mu_B=1$) for $n_s=n_{ovr}=40$ and $n_f=10$ for parallel (full line) and antiparallel (dashed line) configurations. The other parameters as in Fig. 1(c). Thick vertical lines mark the interfaces.

bigger. This is shown in Fig. 3 and, to our knowledge, has not been discussed so far, although such a trend could be predicted on the basis of analytical formulas of Ref. 14. In fact, this finding means that in order to avoid undesirable effects of cap layers (which may be of different thickness in an experiment) on the IEC oscillations one should work with thick magnetic sublayers. It is also noteworthy that the oscillation bias value depends on the magnetic layer thickness, as could be predicted from Eq. (1).

Finally, in connection with the quantum-well state concept,[16–19] we have studied the distribution of induced magnetic moments in the CL (and in the spacer). A typical result is presented in Fig. 4. The induced magnetic moments are measured in dimensionless units ($\mu_B=1$) and are of the order of 0.1% with respect to the magnetic layer magnetization. As expected, the period of the induced-moment distribution within the CL is exactly that anticipated for the bulk CL material FS. The effect of the other sublayers is minor, except that the magnitude of the induced moments is also magnetic-slab dependent. This might seem, at a first glance, to be in conflict with the IEC behavior, which shows no oscillations for the parameters of Fig. 4 [cf. Fig. 1(c)]. Yet the spin polarization in nonmagnetic layers is related to just one system with the fixed sublayer thicknesses and the given alignment of magnetic sublayers, whereas the IEC results from the total energy (thermodynamic potential) balance between the two possible ferromagnetic layer alignments and has to do with the series of samples with changing CL thicknesses. This observation implies that the induced magnetic moments in the nonmagnetic cap layer (as well as the QWS) give in general the whole set of periods, of which only those survive, as far as the IEC is concerned, that fulfill the selection rules referring to the entire system. In other words, the IEC oscillations are the global characteristic of the whole system, whereas the induced spin polarization in the cap layer is strictly of local nature.

The selection rules completed herein by the extra condition related to the extremal spanning vectors of the magnetic sublayers are quite general and apply to real systems too. In particular they allow one to explain why in the case of the Cu/Co/Cu/Co multilayer the short period of oscillations with Cu cap-layer thickness is absent[11] in spite of theoretical predictions[14] and the photoemission results concerning QWS.[16,17,19] In fact, the explanation is simple and quite analogous to that of Ref. 22 about IEC oscillations as a function of ferromagnetic layer thickness. Of the two in-plane extremal spanning vectors of the Cu Fermi surface only the ''belly'' one (at $\vec{k}_{\parallel}=\vec{0}$) coincides with the extrema of the majority and minority sheets of the Co Fermi surface, giving rise to the long period of oscillations. The ''neck'' spanning vector has no counterpart in the Co FS and this is why there are no short-period oscillations.

V. CONCLUSION

In conclusion, we have shown that in order for the interlayer exchange coupling oscillations versus cap-layer thickness to exist, it is necessary that both the cap-layer and magnetic-layer Fermi surfaces share the same extremal in-plane spanning vectors. If this selection rule is not fulfilled, the period anticipated from the bulk cap-layer material will not occur in the exchange coupling, although it will still be present in the induced moment distribution across the cap layer. Another finding of this paper is that the IEC oscillations versus CL thickness vanish if the magnetic sublayer thickness tends to infinity.

ACKNOWLEDGMENTS

This work has been carried out under the KBN Grants Nos. 2P03B-165-10 (M.Z.) and 2-P03B-099-11 (S.K.). We thank the Poznań Supercomputing and Networking Center for the computing time.

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