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Intrinsic periodicity associated with quantum-well states in a magnetic sandwich

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Abstract. From a simplified quantum-well model for a magnetic sandwich, it can be shown that in the variation of the number of occupied levels with the spacer layers, there exists an intrinsic periodicity, which leads the Fermi level to oscillate periodically. The intrinsic periodicity does not depend on the magnetic alignment but only on the quantum-well states themselves. The oscillation period can be approximately given by $T = (1/\beta)\sqrt[3]{\pi\mu_{\parallel}/(3n_0\mu_{\perp})}$, where $\mu_{\parallel}$ and $\mu_{\perp}$ are the effective masses of the electron in the lateral and perpendicular directions respectively, β is the distance between the two neighbouring atomic layers, and n_0 is the electron density in the spacer layers. This makes one speculate that the long periodicity of the oscillatory coupling could be a result of the intrinsic periodicity, if $\mu_{\parallel}/\mu_{\perp} \gg 1$ and a small s-electron density are assumed. On the other hand, from the calculated energy bands for a thin film, it is found that the electronic structure is highly anisotropic, which is in agreement with this assumption. Therefore, it can be confirmed that the intrinsic periodicity plays an important role in the oscillatory coupling. An inverse photoemission experiment on Cu(100) films over Co can be explained quite well using this physical picture.

1. Introduction

The discovery of oscillatory interlayer coupling in a magnetic metallic superlattice [1–4] has stimulated a great effort to seek its origin experimentally [5–19] and theoretically [20–33]. Historically, a similar effect has been observed as an indirect interaction between a pair of isolated magnetic impurities embedded in a metal. This has led to the belief that the two phenomena may have a common origin, the Ruderman–Kittel–Kasuya–Yosida interaction [26, 34, 35]. However, the big discrepancy in the oscillation period between the theoretical prediction and the experiment has been a puzzle. Furthermore, inverse photoemission experiments [14, 18] have shown that it may be caused by the quantum-well states. Thus, theoretically, how to explain it in terms of the quantum-well states is of interest [22, 33]. According to earlier investigations, from the quantum-well model [22, 33], following the basic idea of the RKKY mechanism, it is also possible to show that spin-polarized quantum-well states could lead to the ferromagnetic layers being coupled oscillatorily.

Nevertheless, there exist many important differences between the quantum-well model and the original RKKY model, as detailed below.

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(1) For a very thin film, there is a quantum-size effect [36]. The electronic structure itself, which includes the eigenvalues of the discrete quantum-well states, the number of electrons and the number of occupied levels, may change with the spacer layers. This was not considered in the previous RKKY theory [26].

(2) The Heisenberg interaction between the neighbouring magnetic atoms prevents the s–d spin-flip scattering process. Thus, the spin-polarization effect of the ferromagnetic layers is stronger than that of magnetic impurities, which can lead to bound-electron states even in a free-electron gas [37].

In [36], the quantum-size effect in a metallic thin film was investigated thoroughly. In that paper, the authors assumed that the Fermi energy was a constant, as it was in the bulk and did not change with the thickness of a thin film. They showed that in this case the electron density would oscillate with the thickness. In the earlier quantum-well model [22], the quantum-size effect was not investigated, and also a constant Fermi energy was assumed. In this paper, the quantum-size effect in the oscillatory coupling will be investigated. The electron density is assumed to be a constant and does not change with the thickness of a thin film. A new effect, the oscillation of the Fermi surface, will be presented; this can affect the period of the spin-polarized energy of the multilayers. This effect is found to be mainly caused by the quantum-size effect, so it is independent of the magnetic alignment of ferromagnets.

The arrangement of this paper is as follows. In section 2, a simplified quantum-well model will be introduced. In the following two sections, the intrinsic periodicity of the Fermi energy with spacer layers will be given. In section 4, the influence of the lattice potential will be investigated in terms of the energy band theory. In section 5, the inverse photoemission experiment will be discussed. Finally, some conclusions will be given.

2. A simplified quantum-well model

The magnetic sandwich used here contains two ferromagnets, each having a thickness c, which is equivalent to $P_x/2$ monolayers, separated by a metal spacer of thickness $2b$, which is equivalent to L_x monolayers. The distance between the two monolayers is β for both of the ferromagnets and the spacer.

In the perpendicular direction, the translational symmetry is broken, which makes the electron energy spectrum different in the two directions. The main differences are as follows.

(1) The boundary conditions of the wave function lead to the discrete energy levels in the perpendicular direction.

(2) Because of the potential missing from sites outside the surface, the variation of the electron potential energy in the perpendicular direction is different from that in the lateral direction. In the latter case, it can be approximately considered as a constant. However, in the first case, it changes with the location and is higher near the surface than it is in the middle.

(3) The ferromagnets will further affect the eigenvalues of an electron in the perpendicular direction through the mismatch of the wave function at the ferromagnet/spacer interfaces. The energy modification depends on the magnetic alignment and electron spin. The effect of the ferromagnetic slabs on the electron gas can be attributed to the spin polarization.

In order to investigate the variation of the electronic structure with the spacer layers and considering factor (1), a quasi-one-dimensional infinite potential well is used. The width

of the potential well is equal to the thickness of the sample, $2a = 2b + 2c$, equivalent to N_x monolayers. The perpendicular direction is denoted as the x-direction and the film surface is in the yz-plane. Considering factor (2), $\mu_\parallel/\mu_\perp \gg 1$ is assumed. For our purpose, the quantum-size effect will be given more emphasis than the spin-polarization effect. The ferromagnetic slabs are replaced by two magnetic monolayers, which are located at the interfaces. The standard s–d interaction Hamiltonian is used and, considering the Heisenberg interaction between the nearest-neighbouring magnetic atoms, the s–d spin-flip process is neglected.

The Hamiltonian of a simplified quantum-well model can be written as follows [33]:

$$\hat{H}_0 = -\frac{\hbar^2}{2\mu_\perp}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\hbar^2}{2\mu_\parallel}\left(\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{\mathrm{d}^2}{\mathrm{d}z^2}\right) \tag{1}$$

$$\hat{H}_{s-d} = \pm[V_2\delta(x+b) + V_1\delta(x-b)] \tag{2}$$

where $V_1 = -JS_1^z\beta$ and $V_2 = -JS_2^z\beta$; J is the exchange integral constant; S_1^z and S_2^z are the spin operators of the magnetic moments for the ferromagnets on the left- and right-hand sides respectively; the positive sign is for an electron with spin up and the negative sign is for an electron with spin down.

The eigenvalue of the Schrödinger equation can be written as

$$\varepsilon_{\boldsymbol{k}} = \hbar^2 k_x^2/(2\mu_\perp) + \hbar^2(k_y^2 + k_z^2)/(2\mu_\parallel).$$

The eigenvalue equations for k_x for a ferro- and an antiferromagnetic coupling can be obtained by a quantum mechanism [33]. For the sake of convenience, they are listed as follows. For a ferromagnetic coupling, there are two equations, one for even and the other for odd parity:

$$\cos k_x a = \mp\frac{2\mu_\perp V_1}{\hbar^2 k_x}\cos(k_x(a-b))\sin k_x b \tag{3}$$

$$\sin k_x a = \mp\frac{2\mu_\perp V_1}{\hbar^2 k_x}\sin(k_x(a-b))\sin k_x b \tag{4}$$

and for antiferromagnetic coupling:

$$\sin 2k_x a = \left(\frac{2\mu_\perp V_1}{\hbar^2 k_x}\right)^2 \sin^2(k_x(a-b))\sin 2k_x b \tag{5}$$

where the negative sign is for spin up and the positive sign for spin down.

(1) Because $|2\mu_\perp V_1/(\hbar^2 k_x)| \ll 1$, the eigenvalues can be separated as $\varepsilon_{n,\sigma} = \varepsilon_n^0 + \Delta\varepsilon_{n,\sigma}$, where ε_n^0 is the unperturbed one and $\Delta\varepsilon_{n,\sigma}$ is the spin-polarized one.

(2) For a ferromagnetic alignment, $\varepsilon_{n,\uparrow}$ is different from $\varepsilon_{n,\downarrow}$. This makes the electron level split, and the gap is proportional to V_1, which is given by

$$\begin{aligned} \Delta\varepsilon_{n,\uparrow} &\approx \frac{2V_1}{a}\sin^2\frac{cn\pi}{2a} \\ \Delta\varepsilon_{n,\downarrow} &\approx -\frac{2V_1}{a}\sin^2\frac{cn\pi}{2a} \qquad n = 1, 2, \ldots. \end{aligned} \tag{6}$$

(3) For an antiferromagnetic coupling, the modification is independent of spin, which can be expressed as

$$\Delta\varepsilon_n \approx \frac{8\mu_\perp V_1^2}{\hbar^2 n\pi}\sin^3\frac{cn\pi}{2a}\cos\frac{cn\pi}{2a} \qquad n = 1, 2, \ldots. \tag{7}$$

(4) The spin-polarized energy which depends on the ferromagnetic alignment is expressed as

$$W = \frac{\mu_\parallel}{4\pi\hbar^2}\sum_{n=1}^{m}\sum_{\sigma=1,2}[E_f^2 - \varepsilon_{n,\sigma}^2] \tag{8}$$

where E_f is the Fermi energy, which will be discussed in detail in the next section.

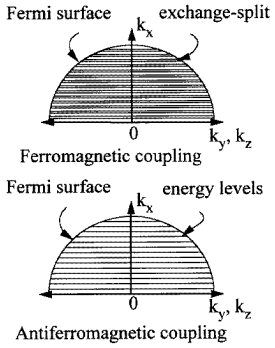

Figure 1. The structure of the Fermi surface for an electron gas in a magnetic sandwich; the upper panel is for a ferromagnetic coupling, in which the exchange splitting has been shown; the lower panel is for an antiferromagnetic one.

3. The number of occupied levels and the Fermi energy

In a simplified quantum-well model, at $T = 0$ K, the momentum in the x-direction is a scale quantity and quantized, and in other directions it is continuous; this can be viewed in momentum space, as shown figure 1. The top panel of the figure is for a ferromagnetic coupling, while the lower panel is for an antiferromagnetic one.

The Fermi surface is a constant-energy surface which separates the unoccupied from the occupied region of k-space, which can be described by the upper part of an ellipsoid surface, the symmetrical axis being fixed in the k_x-direction. The long axis is in the $k_x = 0$ plane and its radius is $\tilde{k}_{n,\sigma} = \sqrt{2\mu_\parallel E_f/\hbar^2}$, and the maximum kinetic energy is at the brim, which is given by $\tilde{\varepsilon}_{n,\sigma}$; the short axis is in the k_x-direction, and its magnitude is $\sqrt{2\mu_\perp E_f/\hbar^2}$. Every occupied level can be thought of as a two-dimensional electron gas and is represented by a disc, which is normal to the k_x-axis; the k_x-coordinate of the disc is $k_{n,\sigma}$, which is evenly distributed between 0 and $\sqrt{2\mu_\perp E_f/\hbar^2}$.

For an occupied level n, σ, since $E_f = \varepsilon_{n,\sigma} + \tilde{\varepsilon}_{n,\sigma}$, it follows that

$$E_f = \frac{1}{2m}\sum_{n=1}^{m}\sum_{\sigma=1}^{2}(\varepsilon_{n,\sigma} + \tilde{\varepsilon}_{n,\sigma})$$

where m is the number of occupied levels.

The total number of electrons, N_e, can be expressed in terms of $\tilde{\varepsilon}_{n,\sigma}$ as

$$N_e = [S/(2\pi)]\sum_{n=1}^{m}\sum_{\sigma=1}^{2}\int_0^{\tilde{k}_{n,\sigma}} k_\parallel \, \mathrm{d}k_\parallel = [S\mu_\parallel/(2\pi\hbar^2)]\sum_{n=1}^{m}\sum_{\sigma=1}^{2}\tilde{\varepsilon}_{n,\sigma}$$

where S is the area of the sample and $S\mu_\parallel/(2\pi\hbar^2)$ is the density of states (DOS) for a level. On the other hand, viewing in a real space, $N_e = 2n_0\beta[L_x + \rho P_x]$, where n_0 is the electron

density of the spacer for two spins and ρn_0 is that of the ferromagnetic slabs. Thus, the Fermi energy is found as

$$E_f = \frac{2\pi\hbar^2 n_0\beta}{m\mu_\parallel}[N_x - (1-\rho)P_x] + \frac{\pi^2\hbar^2(m+1)(2m+1)}{12\mu_\perp\beta^2 N_x^2} + \frac{1}{2m}\sum_{n=1}^{m}\sum_{\sigma}^{2}\Delta\varepsilon_{n,\sigma}. \tag{9}$$

The number of occupied levels can be determined in terms of $\varepsilon_m^0 \leqslant E_f \leqslant \varepsilon_{m+1}^0$. It can be shown that the summation of the last term on the right-hand side is much smaller than the other terms and can be neglected. So, in a first approximation, the Fermi energy is, in fact, independent of the alignment of the ferromagnets. Thus, it becomes a simple electronic state problem in a quantum-well model [38].

If one lets $T = (1/\beta)\sqrt[3]{\pi\mu_\parallel/(3\mu_\perp n_0)}$, $c_0 = (1-\rho)P_x$, then

$$E_f(N_x, m) = \epsilon_f\left[\frac{2}{3}\frac{N_x - c_0}{mT} + \frac{(m+1)(m+1/2)}{3}\left(\frac{T}{N_x}\right)^2\right] \tag{10}$$

where

$$\epsilon_f = \frac{\pi^2\hbar^2}{2\mu_\perp\beta^2T^2}.$$

The minimum of E_f is determined by the conditions $\partial E_f/\partial N_x = 0$ and $\partial^2 E_f/\partial N_x^2 > 0$, from which one finds

$$N_x(m) = T\sqrt[3]{m(m+1)(m+1/2)} \approx T\left(m + \frac{1}{2} + \frac{1}{12m}\right) + \mathrm{O}(T/m^2)$$
$$\Delta N_x = N_x(m+1) - N_x(m) = T + \mathrm{O}\left(\frac{T}{12m(m+1)}\right).$$

On the other hand, the thickness for the discontinuity of $\partial E_f/\partial N_x$ is determined by the condition $E_f(N_x, m) = E_f(N_x, m+1)$, from which one finds

$$N_x(m) = T\left[m + \frac{3}{4} + \frac{c_0}{3T} + \frac{1}{m}\left(\left(\frac{c_0}{3T}\right)^2 - \frac{7}{48}\right)\right] + \mathrm{O}(T/m^2)$$
$$\Delta N_x = N_x(m+1) - N_x(m) = T + \mathrm{O}\left(\frac{T}{m(m+1)}\left[\left(\frac{c_0}{3T}\right)^2 - \frac{7}{48}\right]\right).$$

Therefore, from the thickness variation of the minimum of E_f and the discontinuity of $\partial E_f/\partial N_x$, one can conclude that both the Fermi energy and the number of occupied levels are oscillatory functions of the thickness and T is the oscillation period.

Because $\varepsilon_m^0 < E_f < \varepsilon_{m+1}^0$, the oscillation amplitude can be found as

$$A_f = \varepsilon_{m+1}^0 - \varepsilon_m^0 \approx \frac{1}{m\mu_\perp}\left(\frac{\pi\hbar}{\beta T}\right)^2. \tag{11}$$

So the fluctuation of the Fermi energy with N_x is proportional to $1/N_x$. If m becomes large enough, the amplitude approaches zero. Consequently, the Fermi energy will be a constant and $E_f = \epsilon_f$. In this case, one can compare the Fermi energy with that of the three-dimensional electron gas models directly. For a thin film, the Fermi energy can be rewritten as

$$\epsilon_f = \frac{\hbar^2(3\pi^2 n_0)^{2/3}}{2\mu_\perp^{1/3}\mu_\parallel^{2/3}}.$$

For the three-dimensional electron gas, $\mu_\parallel = \mu_\perp = \mu_e$ and the Fermi energy and the wave vector are E_f^0 and k_f respectively. From $E_f^0 = \hbar^2 k_f^2/2\mu_e$ and $n_0 = k_f^3/(3\pi^2)$, one obtains two important relations:

$$T = \frac{\pi}{\beta k_f}\sqrt{\frac{\mu_e}{\mu_\perp}} = \frac{\pi}{\beta k_f}\frac{\mu_\parallel}{\mu_e} \qquad \text{and} \qquad \mu_\perp \mu_\parallel^2 = \mu_e^3\left(\frac{E_f^0}{E_f}\right)^3. \tag{12}$$

Because the RKKY oscillation period is $T_{RKKY} = \pi/(\beta k_f)$, the oscillation period of the Fermi energy is $\mu_\parallel/\mu_e$ times as much as the RKKY one.

4. Energy band theory

It has been shown that a magnetic sandwich has an intrinsic periodicity and that the period depends on the ratio of the effective masses in two directions. If the oscillatory coupling has the same origin as the intrinsic periodicity, then $\mu_\parallel/\mu_\perp \gg 1$ and a small electron density n_0 should be expected. However, where does the high anisotropy come from? It is difficult to understand and seems impossible to find the solution from such a simple model. The reason may be that the lattice potential has been neglected. Its effects and the origin of the anisotropy should be explained in terms of the energy band theory.

Because the translational symmetry is broken in the perpendicular direction, plus the boundary conditions, the special effect of the lattice potential should be considered. The potential missing from sites outside the surface is equivalent to adding a strong electric field, pointing from the centre to the outside. The electric field makes the electron potential energy higher on the surface than it is in the middle. Consequently, the electronic structure of a thin film differs from that of a bulk in the following three ways.

(1) In the perpendicular direction, the eigenvalues of the discrete levels and the gaps between the two neighbouring levels become larger than they are in an infinite potential well. As a result, the assumption that $\mu_\perp \ll \mu_e$ should be reasonable.

(2) Because the eigenvalues of discrete levels increase, the number of occupied levels should be reduced and the electron population in each occupied level increases. This causes the Fermi wave vector in the lateral direction to expand outside. Because of the degeneracy perturbation by the lattice potential, the kinetic energy will deviate from the square dispersion relation when its wave vector is close to the Brillouin zone boundary. Consequently, the DOS in this direction becomes much larger. Equivalently, one can expect $\mu_\parallel/\mu_e \gg 1$.

(3) The electric field induces the first excited states of the Cu atom, the 4p level, to split, leading some of the p-like energy bands to lower to below the Fermi level. Thus, the DOS for p-like electrons on the Fermi surface becomes much larger and the s-like electron density reduces.

If the above analysis is correct, then we can be sure that the lattice potential plays an important role in the origin of the long periodicity. Hence, a further analysis in terms of the energy band theory is necessary, which can provide a touchstone. For simplicity, the effect of the ferromagnetic slabs is neglected and the energy bands of a sandwich are simply replaced by that of a Cu thin film. The energy bands of both Cu thin-film [39–41] and bulk material [42] are available, as they have been calculated by several authors. The energy bands of 19-layer Cu(100) films calculated by Euceda *et al* [40] will be used for analysis. The energy band of bulk Cu calculated by Segall [42] will be used for comparison. Since the Fermi energy is only affected by the occupation of the sp bands, the following discussion will be limited to them. The main characteristics which may be associated with the long periodicity are summarized as follows.

(1) In the perpendicular direction, the electron energy is discrete and in the lateral direction it is continuous. Thus, the discrete levels are described by the states in the one-dimensional Brillouin zone and the number of states is equal to the number of atomic layers. In the lateral direction, the energy bands are described by the two-dimensional Brillouin zone (2D BZ). Since the dispersion relations in the 2D BZ for each of the levels are different, each 2D BZ is connected to only one level.

(2) There are three groups of energy bands which cross the Fermi surface:

(a) $\bar{\Delta}_1$ bands (from $\bar{\Gamma}$ to $\bar{X}$);
(b) $\bar{\Sigma}_1$ bands (from $\bar{\Gamma}$ to $\bar{M}$);
(c) $\bar{Y}_1$ and $\bar{Y}_2$ bands (from $\bar{X}$ to $\bar{M}$).

The gaps between two neighbouring bands depend on what the bands are and their locations. The gaps at the $\bar{\Gamma}$ axis are much larger than those at $\bar{X}$.

(3) The dispersion relation for the energy bands is very complex and the description of the effective mass is not suitable. Nevertheless, the comparison of the width of the energy bands and the Fermi wave vectors between a thin film and a bulk can provide the necessary information for establishing the DOS of each level.

(a) The width of $\bar{\Delta}_1$ bands is from about 2 to 2.9 eV for the lateral direction and 4.5 eV in the perpendicular (100) direction, whereas the width of the Δ_1 band for the bulk (from Γ_{12} to $X_{4'}$) is about 6.1 eV.

(b) The width of $\bar{\Sigma}_1$ bands is about 3.7 eV for a film whereas that of the Σ_1 band (from Γ_{12} to K_1) is 9.45 eV for Cu bulk.

(c) The Fermi wave vector in the (100) direction is $1.0k_{BZ}$ for a film whereas it is $0.79k_{BZ}$ for the bulk, where $k_{BZ} = 2\pi/a_0$.

(d) The Fermi wave vector in the (110) direction is $1.25k_{BZ}$ for a film whereas it is $0.85k_{BZ}$ for the bulk.

From the above comparisons, qualitatively, $\mu_\parallel/\mu_\perp \gg 1$ is correct.

(4) The values for $\bar{Y}_1$ and $\bar{Y}_2$ bands for a film are much lower than the corresponding ones for Σ_3 (p-like) for the bulk. Besides this, all of these bands cross the Fermi surface, are occupied and are close to each other. They provide a very high DOS on the Fermi surface. According to the calculation of the DOS, the crystal configuration for 19-layer Cu(100) films is $3d^{9.89}4s^{0.33}4p^{0.79}$ whereas the atomic configuration is $3d^{10}4s^1$. When the number of atomic layers increases, though both the number of electrons and the number of energy bands increase, it can be expected that the dispersion for each band and the occupation will not change too much. To a very good approximation, when one is considering the number of occupied levels and the Fermi energy to vary with the thickness of the film, the effect from the slowly changing $\bar{Y}_1$ and $\bar{Y}_2$ bands and 4p electrons can be neglected.

From the above energy band analysis, one can draw two conclusions: (a) the density of states in the lateral direction is much larger than it is in the perpendicular direction; and (b) the electron density for the s electron, which is responsible for the oscillation of the Fermi energy, greatly reduces.

In order to give a quantitative estimation for the oscillation period, according to [40], one can take the density of the s electron as n_0 in our quantum-well model, which is only one third of the value for the bulk. Consequently, following the free-electron model, the Fermi wave vector of a bulk can be calculated as $k_f = (3\pi^2 n_0)^{1/3} = 0.79(1/3)^{1/3} = 0.55k_{BZ}$. From the energy band calculation, the Fermi wave vector in the lateral direction can be estimated as $k_F = 1.1k_{BZ}$. If the Fermi energy is the same for the two systems, then $\mu_\parallel/\mu_e = (k_F/f_f)^2 = 4$, from which the period is found to be $T \sim T_{RKKY}(\mu_\parallel/\mu_e) \sim$

$4T_{RKKY}$. Therefore, the speculation regarding the long periodicity is reasonable as regards the physics.

5. The explanation of the inverse photoemission experiment

The inverse photoemission spectra for Cu on Co obtained by Ortega and Himpsel (see [18]) showed that the photoemission intensity at E_f oscillated with the numbers of Cu layers periodically, and that the oscillation period was nearly the same as that of the oscillatory coupling in a magnetic sandwich of Co/Cu/Co. This is the first time that it has been shown that there is a connection between the oscillatory coupling and the quantum-well states from an experiment. An explanation of the oscillatory photoemission intensity at the Fermi energy E_f would be of interest. Originally, on the basis of a study of the bulk band structure, the authors of [18] suggested that (1) the oscillatory intensity at E_f could be due to the modulation of the fast-oscillating Bloch wave by an envelope function, and that the k-vector of the latter is given by the difference between the Fermi wave vector k_f and the wave vector of the Brillouin zone boundary, k_{BZ}; and (2) the origin of the quantum-well states lay in the spin-dependent boundary conditions at the interface with the ferromagnet, and that thus only minority-spin quantum-well states could form at the Fermi level for the x-direction since the majority-spin conduction electron states in the spacer could be coupled to the majority-spin states in ferromagnet.

In this section, it will be shown that the same experiment can be explained in terms of an intrinsic period of the quantum-well states. As a result of the bremsstrahlung effect [43], the inverse photoemission intensity not only depends on the density of unoccupied states at energy E_{final}, but also depends on the energy difference between the initial energy of the captured electron, E_{init}, and E_{final}. In the bulk, the Fermi energy is a constant and can be referred to as a fixed point.

In terms of a simplified quantum-well model, the quantum-well states are assumed to arise from the structure confinement of the sandwich sample, but not from the potential difference at the interfaces. From the last two sections it has been shown that the Fermi level is not a constant; thus it cannot be used as a bonding energy reference level in photoemission measurements; furthermore the Fermi energy itself is an oscillating function of the number of spacer layers. In order to explain the experiment, the quantum-well states in the Cu overlayers on the ferromagnetic layer should be established beforehand. They can be obtained in the same way as before. The width of the quantum well is a, with $a = b + c$, where b and c are the thicknesses of the Cu and Co layers respectively. The s–d interaction Hamiltonian is written as

$$H_{s-d} = \pm V_0\,\delta(x - b) \tag{13}$$

where $V_0 = -S^z J_0 \beta$; the positive and negative signs have the same definition as in equation (2).

The eigenfunction is assumed to be

$$\Psi(x) = \begin{cases} B_1 \sin k_x x & 0 \leqslant x \leqslant b \\ B_2 \sin k_x (x - a) & b \leqslant x \leqslant a. \end{cases} \tag{14}$$

From the connection conditions

$$\begin{aligned} &B_1 \sin k_x b = -B_2 \sin k_x c \\ &B_2 \cos k_x c - B_1 \cos k_x b = \pm \frac{2\mu_\perp V_0}{\hbar^2 k_x} B_1 \sin k_x b \end{aligned} \tag{15}$$

one can derive

$$\sin k_x a = \pm \frac{2\mu_\perp V_0}{\hbar^2 k_x} \sin k_x b \sin k_x c. \tag{16}$$

On comparing equation (16) and equation (4), the quantum-well states in the Cu overlayer are seen to be exactly the same as those of odd parity in a sandwich with ferromagnetic coupling. Therefore, the spin splitting also occurs in these levels, as observed in many photoemission experiments.

From the eigenvalues, the Fermi energy is found as

$$E_f = \frac{1}{m_e}\left[\frac{2\pi\hbar^2\beta n_0}{\mu_\parallel}(L_x + \rho P_x) + \sum_{n,\sigma} \varepsilon_{n,\sigma}\right] \tag{17}$$

which is the same as in equation (9).

Because there is only one ferromagnet, the oscillation behaviour of the Fermi energy arises from the periodicity of the quantum-well states. Therefore the oscillation of the Fermi energy is a general characteristic of the thin film.

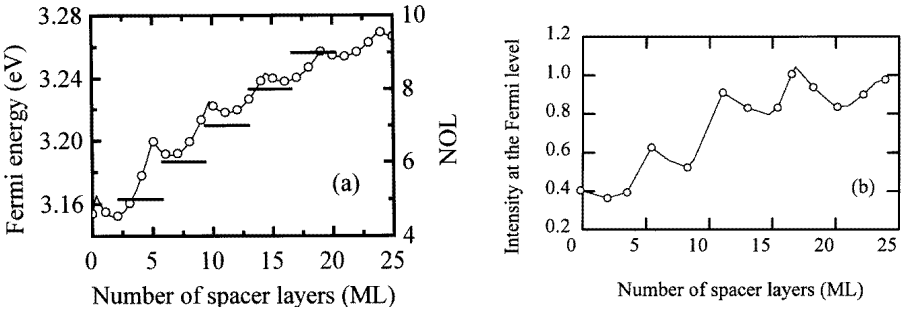

Figure 2. (a) The Fermi energy, on the left-hand axis, and the number of occupied levels (NOL), on the right-hand axis, as functions of the number of spacer layers; the open circles stand for the locations of the spacer monolayers. In this figure, the density of the s electrons is $n_0 = \frac{1}{3}(4/a_0^3)$, $\mu_\parallel/\mu_e = 2.55$ and $\mu_\perp/\mu_e = 0.154$, the period is $T = 4.71$ monolayers, and $P_x = 24$ monolayers. (b) The inverse photoemission intensity at the Fermi energy level for a Cu/Cu sample, shown as a function of the number of spacer layers; the intensity is in arbitrary units [18].

Because the Fermi energy is not a constant, the photoemission intensity will sensitively depend on its variation and it should not be used as a reference point for measurements. Therefore, the period variation in the observed inverse photoemission intensity is mainly caused by the period variation of the Fermi energy.

The Fermi energy and the number of occupied levels as functions of the number of spacer layers are shown in figure 2(a). According to the energy band theory, the density of the 4s electron is 0.33 per atom, so $n_0 = \frac{1}{3}(4/a_0^3)$. If $\mu_\parallel/\mu_e = 2.55$ is assumed and, following the second expression in equation (12), $\mu_\perp/\mu_e = 0.154$, the period is $T = 4.71$ monolayers. $P_x = 24$ monolayers and $\rho = 0.24$ are assumed.

For a comparison, the inverse photoemission intensity at the Fermi energy level for a Cu/Cu sample is shown in figure 2(b).

6. Conclusions

Using a simplified model, the intrinsic periodicity associated with the quantum-well states both in a magnetic sandwich structure and in a sample containing only a ferromagnet with

an overlayer is investigated. It is found that this periodicity should be completely attributed to the quantum-well states themselves but not to the ferromagnets. The reason for this is that the values of the discrete levels are inversely proportional to the square of the width of the quantum well, which is weakly affected by the existence of the ferromagnet, and the number of electrons must be proportional to the well width; in order to keep the total energy at a minimum, the number of occupied levels is forced to increase with the well width in a periodic way. The periodic behaviour of the number of the occupied levels leads the Fermi energy to change periodically too. The period is given by $T = (1/\beta)\sqrt[3]{\pi\mu_{\parallel}/(3n_0\mu_{\perp})}$. According to the energy band theory of thin film, it is found that the effects of the lattice potential of the thin film can result in the electron DOS being highly anisotropic in the two directions and the number of s electrons reducing. Qualitatively, the energy band effects of the thin film are responsible for the long periodicity of the Fermi energy oscillation. One can use this result to explain the inverse photoemission intensity at the Fermi energy level, which is oscillatory with spacer layers.

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