The influence of effective mass
on magnetoresistance in ultrathin Fe/Cr/Fe films

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The transport properties of ultrathin metallic sandwich structures of Fe/Cr/Fe are studied as a function of magnetic layer thickness for the current in plane geometry (CIP). Taking into account the band structure obtained from density functional theory (DFT), we calculate basic physical properties such as Fermi energy and relaxation time for each magnetic and spacer layer. Next, using the Boltzmann formalism in its extended form, we obtain results for magnetoresistance (MR). In particular, we analyse the influence of effective mass parameterisation.

Key words: *magnetoresistance; multilayer; Boltzmann equation; effective mass of electrons*

1. Introduction

Progress in the fabrication of very thin magnetic layers separated by non-magnetic films has led to the discovery of giant magnetoresistance (GMR). This effect was originally discovered in Fe/Cr/Fe multilayers [1, 2]. GMR is the change of electrical resistance observed when rotating from an antiparallel to parallel alignment of film magnetizations. For its description, two different approaches are usually used: the quasi-classical method based on the Boltzmann equation [3–5] or the quantum -mechanical Kubo formalism [6].

Most of models are idealized and do not take into account the details of the materials or the finite sample size. It is a well known fact that for a very thin layer the basic physical quantities connected with transport, such as the Fermi energy, effective mass, and relaxation time of electrons, depend on the boundary conditions at the surface. A precise description of transport in such a system is very important from the technological point of view, but requires a proper set of parameters describing the multilayered structure to be determined.

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In our earlier work [7], we have determined the electronic structure and layer potentials in a Fe/Cr/Fe trilayer, as well as the Fermi energy characterizing the system. These data are used in the present paper to determine the effective mass of electrons and to analyse its influence on GMR.

2. Model description

A proper choice of potentials for the trilayer plays a very important role in GMR calculations. The electronic structure, as well as the magnetic properties of the $Fe_N/Cr/Fe_N$ trilayer (N is the number of atomic layers) have been widely studied using density functional theory (DFT) in the local spin approximation [7]. We consider the transport properties in magnetic multilayers for electronic current in the layers parallel to the surface of the sample.

GMR is then determined by the relation $MR = \left(\sigma_{\uparrow\uparrow} - \sigma_{\uparrow\downarrow} \right) / \sigma_{\uparrow\uparrow}$, where the conductivity of the trilayer sample is given by the formula

$$\sigma_{\uparrow,\uparrow(\downarrow)} = \frac{1}{d} \sum_{\sigma v} \int_{(v-1)a}^{va} \sigma_{\uparrow,\uparrow(\downarrow)}^{v\sigma}(z) dz \tag{1}$$

for the parallel $\sigma_{\uparrow\uparrow}$ or antiparallel $\sigma_{\uparrow\downarrow}$ configurations of magnetization in iron layers, while in terms of the Hood and Falicov approach the local conductivity can be introduced in the form

$$\sigma_{\uparrow,\uparrow(\downarrow)}^{v\sigma}(z) = -e^2 \left(\frac{m_\sigma^*}{h} \right)^3 \tau_{v\sigma} \int d^3 \upsilon \left(\upsilon^x \right)^2 \frac{\partial f_{v\sigma}^0}{\partial E_\sigma^{\uparrow,\uparrow(\downarrow)}} \left(1 + F_\sigma^{\uparrow,\uparrow(\downarrow)}(\upsilon) e^{\mp \frac{z}{\tau_{v\sigma}|\upsilon^z|}} \right) \tag{2}$$

where the symbols have their usual meanings as described in [8].

Besides fundamental quantities such as electron charge and Planck's constant, we need to determine the effective mass of the electron m_σ and the relaxation time $\tau_{v\sigma}$ considered in each monatomic layer. DFT calculations allow us to obtain these constants on the basis of the electronic structure of a sample by means of the density of states and the Fermi level, which determines the effective potentials for electrons with oriented spins.

The conductivity given by (2) is derived using the semi-classical Boltzmann equation for the distribution function $f_{v\sigma} = f_{v\sigma}^0 + g_{v\sigma}$, where $f_{v\sigma}^0$ is the equilibrium distribution function for electrons with spin σ appearing in the layer v in the absence of any electric field E, while $g_{i\sigma}$ contributes to the Boltzmann distribution by the influence of the electric field. Next, we can see that we should determine the integral constants $F_\sigma^{\uparrow,\uparrow(\downarrow)}$ appearing in Eq. (2) in a way that allows us to satisfy the matching conditions for the Boltzmann functions $f_{v\sigma}$ at the interfaces between ferromagnetic and

spacer films. The construction of these matching conditions is presented in [9]. The results depend on the specularity factors P_σ, considered at the outer surfaces and connected to surface roughness. In order to extend our considerations to a more realistic case from the physical point of view, we define the specularity factor P_σ using the physical pictures of electrons moving through a potential barrier. In this case, the value of P_σ corresponds to the specularity factor in the Fuchs–Sondheimer [9] conductivity theory of thin films and can be expressed by the effective result

$$P_\sigma = \left(1 - \frac{\left(\chi_F^\sigma\right)^2 \cos^4\theta + 2}{1 + \left(\chi_F^\sigma\right)^2 \cos^4\theta}\right)\left(1 - \frac{\left(\chi_F^\sigma\right)^2 \cos^4\theta + 2}{1 + \left(\chi_F^\sigma\right)^2 \cos^4\theta}\exp\left(-\frac{\dfrac{d}{\tau_\sigma \upsilon^2}}{\cos\theta}\right)\right)^{-1} \tag{3}$$

which is an alternative to other models, assuming that the coefficients for coherent transmission and specular reflections are determined in quantum mechanics by matching free electron wave functions at each interface [10]. The constant χ_F^σ is defined in terms of the Fermi velocity υ_F, where m_σ is the effective mass of electrons and the relaxation time τ_σ is taken for electrons at the surface, i.e. $\tau_\sigma = \tau_{1\sigma}$ or $\tau_\sigma = \tau_{N\sigma}$. This parameter is determined from DFT. From the physical point of view, the constant χ_F^σ represents the ratio of the electron free path and de Broglie wavelength, and is related to the angle of incidence of electrons with respect to the z-axis as $\chi_F^\sigma = \left(2m_\sigma\tau_\sigma\upsilon_F^2\right)/\hbar$. The relaxation time can be evaluated in terms of DFT calculations by means of the Fermi golden rule. The relaxation time can be expressed as follows [11]:

$$\left(\tau_{v\sigma}\right)^{-1} = 2\pi c\rho\left(E_F\right)\left(V_{v\sigma}\right)^2 \tag{4}$$

i.e., it is determined by the parameters of the potential barrier, in particular by the shape of the density of states at the Fermi level. In Eq. (4), c is the number of scattering centres and plays the role of a calibration factor when comparing the obtained relaxation time with the average values discussed in literature [8, 11].

3. Results

The dependence of GMR on the number of ferromagnetic monatomic layers N in a trilayer $Fe_N/Cr/Fe_N$ with a fixed spacer thickness of $d_s = 4.32$ Å is shown in Fig.1 for various effective electron masses. The calculations were performed using the matching conditions $V_M = -8.23$ eV, $V_m = -5.73$ eV, $V_S = -5.77$ eV; V_M, V_m, V_s corresponding to the potential barriers for majority and minority spins in the ferromagnetic layer and the spacer, respectively, and the relaxation time for electrons $\tau = 5\times10^{-13}$ s in the case of the Hood–Falicov approach [8] to describe GMR.
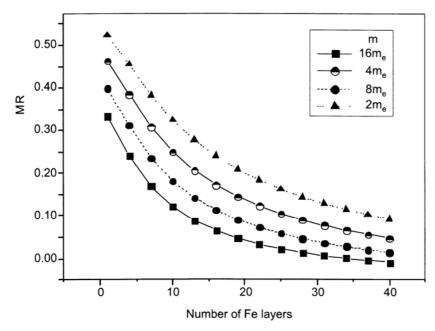
Fig. 1. Ratio of GMR and the number of ferromagnetic monolayers for four effective electron masses. The calculations are based on the theoretical model described in [9], with the following parameterisation: potentials: $V_M = -8.23$ eV, $V_m = -5.73$ eV, and $V_S = -5.77$ eV, relaxation time $\tau = 5 \times 10^{-13}$ s
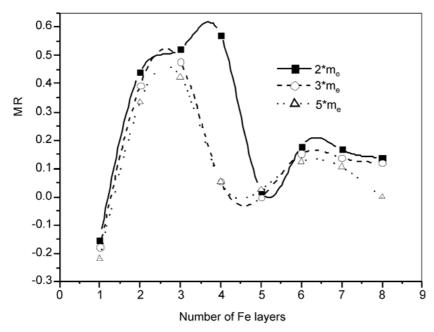

Fig. 2. GMR ratio as a function of the number of ferromagnetic layers for three effective electron masses in the Fe/Cr/Fe trilayer. All the parameters used in calculations were determined from DFT [7]

The GMR results shown in Fig. 2 are obtained for three different effective masses and parameters taken from the DFT calculations. It is worthwhile to notice that the DFT parametrisation curves oscillate with varying amplitude, while the character of these oscillations depends on the effective mass. In particular, when we compare the upper curve in Fig.1 (dotted line), obtained by means of the Hood–Falicov approach ($m^* = 2m_e$), with the curve in Fig. 2 (solid line) for the same effective mass ($m^* = 2m_e$), we can see that the appearance of oscillations is connected to the fact that DFT calculations are used. From the physical point of view, these calculations include band parameterisation as well as the geometry of the considered system. The band structure departs from its quasi-free particle behaviour and the method conserves the shape of the dispersion law, while the effective mass parameterisation now depends on the wave vector distribution, effectively leading to a change in the dispersion law. Thus, the effective mass m^* applied in the case of the Hood–Falicov approach is equivalent to the coefficient $m^*(k = 0)$ appearing in the DFT representation.

In the above context, we can conclude that the most important results obtained in the present paper are the oscillatory character of GMR in $Fe_N/Cr/Fe_N$ with respect to the number of Fe layers and that the source of these oscillations is connected to the shape of the energetic bands, which are described by boundary conditions directly related to the geometry of the considered sample and included immanently in DFT calculations.

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