

Surface contribution to giant magnetoresistance in Fe/Cr/Fe films

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Transport properties of very thin films have been analysed using the layered potentials calculated by means of the *ab initio* method represented by the density functional theory (DFT) in the planar geometry for the $n\text{Fe}/3\text{Cr}/n\text{Fe}$ films, where n is the number of monoatomic Fe layers, ($1 \leq n \leq 8$). We also take into consideration the values of the relaxation time and the effective mass of an electron in terms of the considered potentials. The matching conditions have been applied at the interface and the boundary conditions at the surface in order to determine the contributions to the giant magnetoresistance (GMR) coming from the surface, interface, and inner layers. The surface roughness is introduced by means of the specular factor P_σ defined in the spin-dependent terms responsible for the scattering of the electrons. Thus, the electron scattering at the outer surfaces depends on both spin orientations. The main result obtained in the paper is the evaluation that the surface contribution to GMR is very small in comparison with the effect of interface.

Key words: *multilayers; giant magnetoresistance; conductivity; thin films*

1. Introduction

The giant magnetoresistance (GMR) in multilayers originates from the spin-dependent electron scattering inside a layered structure made of ferromagnetic layers sandwiched between nonmagnetic layers (spacers) and stacked along the direction orthogonal to the layer planes. The electron scattering takes place in each layer, in particular, at non-ideal, rough, and diffusive interfaces and at the outer surfaces of the considered sample [1]. The purpose of the present paper is to investigate the contribu-

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tion to GMR coming from surfaces, interfaces as well as from inner layers and to compare their influence on the total GMR of the Fe/Cr/Fe sample.

Our considerations are based on the relation between the current of electrons moving in the sample in plane of its surface under the influence of an electric field. The conductivity is then given by the derivative of the current with respect to the applied electric field tending to zero in each monoatomic layer. Thus, the conductivity is of a local character, calculated in the bidimensional space for a planar system embedded into the effective field generated by the interaction between the layered systems. In order to calculate the global value for the conductivity, we sum up all the planar contributions in the case of current in plane (CIP) geometry while the case of current perpendicular to plane (CPP) geometry requires the summation over the local values of the resistivity.

The main advantage of the method used here is a formulation the relation between the electronic current and the applied electric field in a way which allows us to use the input database for a given sample without any fitting or parametrisation. As a source for this purpose, we choose the density functional theory (DFT) whose output data collect the set of the energy eigenvalues, eigenfunctions associated to them and local potential barriers in two dimensional space. *Ab initio* calculations of the electronic structure for practical reasons were performed by means of the density functional theory in the local spin approximation (LSDA). The Kohn–Sham equation was solved using the full potential in the representation of linearized augmented plane wave (FP-LAPW) in a slab geometry [2]. The method is extremely advantageous for computing the electronic structure of multilayers because it was designed to take into account the boundary conditions in the slab geometry for the outer layers remaining in contact with vacuum.

2. Method of calculation and the transport model

The calculations were performed for the slab consisting of 3 films, as shown in Fig. 1. The considered systems are made of 3 Cr monolayers (spacer) in antiferromagnetic ordering sandwiched between two films of n Fe monolayers. The magnetization of the ferromagnetic layers is permitted to be parallel or antiparallel depending if an external magnetic field is applied to the sample or not. The electronic structure is calculated within the framework of the DFT approach for each monolayers ν in the trilayered system $n\text{Fe}/3\text{Cr}/n\text{Fe}$ bcc (100) with n ranging from 1 up to 8 monolayers. The method of calculation gives the properties of electronic structures that we use as the input for calculating the transport properties described by our model which is based on the Boltzmann formalism. One of the properties that we are able to calculate with our DFT method is the potential barrier distribution $V_{\nu\sigma}$ in which the charge carriers are embedded. A detailed description and the physical origin of the $V_{\nu\sigma}$ parameter can be found in Ref. [3].

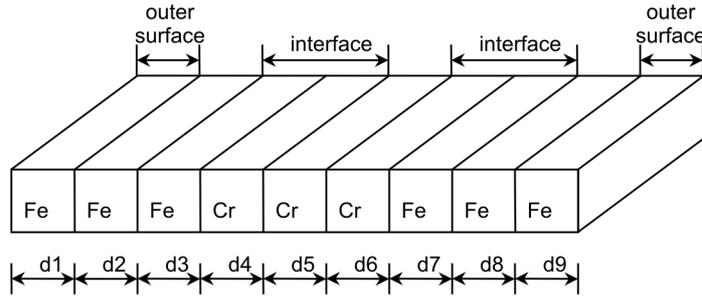


Fig. 1. The structure of the layers for the $(n\text{Fe}|3\text{Cr}|m\text{Fe})$ trilayer system

The potential is different for the electrons with the majority and minority spins in Fe films while for the spacer electrons in Cr film the potential is independent of the spin orientations. The second parameter which is calculated in terms of DFT method is the relaxation time determined by means of the Fermi golden rule [4]

$$(\tau_{v\sigma})^{-1} = \frac{c}{\hbar} \rho_v(E_F) (V_{v\sigma})^2 \quad (1)$$

where $\rho_v(E_F)$ is the local electronic density of states at the Fermi level E_F . The value c appearing in Eq. (1) is known as a concentration of scattering centres and it can be treated as a calibration constant. The calculated local densities of states are given in Ref. [3] were obtained by means of the DFT approach. The relaxation time is then determined by Eq. (1) in each monatomic layer separately in the case of electrons with the spin up and spin down. In our calculations of the transport properties, we also need to know the effective mass m_σ^* which is provided by our spin-dependent band structure method

$$\frac{1}{m_\sigma^*} = \frac{1}{\hbar^2} \left. \frac{\partial^2 E_\sigma(k)}{\partial k^2} \right|_{k=k_F} \quad (2)$$

where E_σ is the s, p electronic band energy. In order to calculate the conductivity of a sample, we use the Boltzmann equation in the relaxation time approximation. The Boltzmann function considered in the direction perpendicular to the surfaces represents the number of charged carriers confined perpendicularly to the surface plane by the boundary conditions which are determined by the specularity factor P_σ [3]

The interfaces are determined by the matching conditions in the sense of the Hood–Falicov treatment [5] for the potential taken from the DFT results for the interfaces at $v \in (n, n+1)$ and $v \in (n+3, n+4)$ (see Fig. 1).

3. Results

In Figures 2 and 3, we show the relaxation time in the ferromagnetic monolayer position ν for both spin orientations σ of the charged carriers. A comparison of the relaxation time calculated in each monoatomic layer ν reveals an evident spin orienta-

tion dependence. The difference between the relaxation times for various systems, e.g. for $n = 7$ (Fig. 2) and $n = 6$ (Fig. 3) is also seen. The relaxation time is usually treated in the semiclassical approach as a constant which does not depend on the spin orientations. Its spin dependence, however, is one of the sources of GMR.

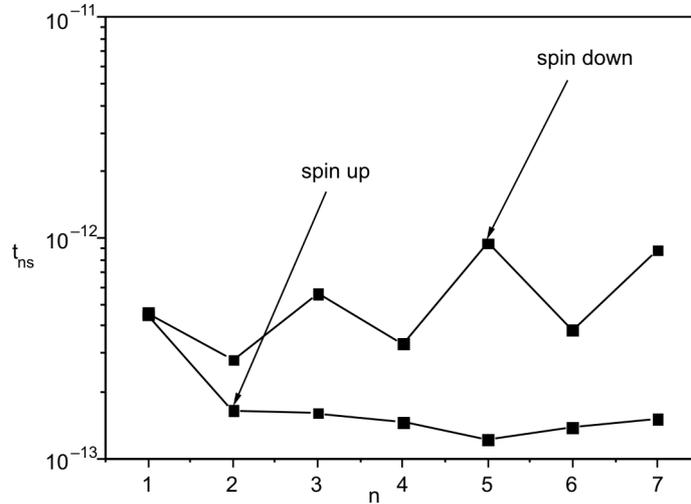


Fig. 2. Description of the relaxation time, $\tau_{\nu\sigma}$ in the monoatomic Fe layer ν ($\nu \in 1, 7$) for the system (7Fe|3Cr|7Fe). The spacer thickness equals 4.33 Å

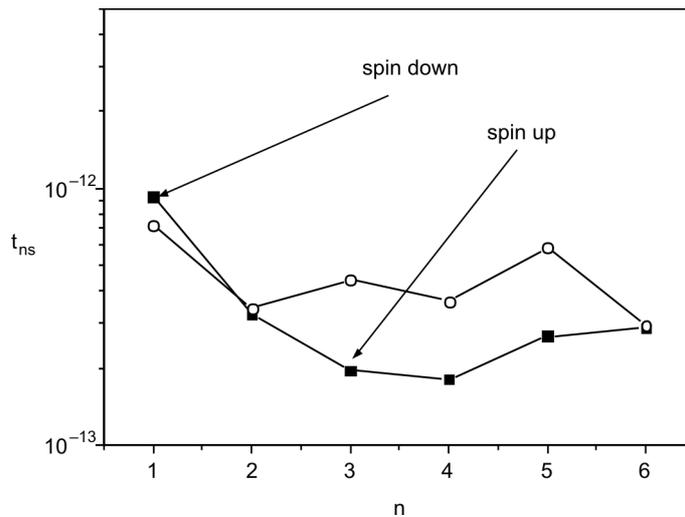


Fig. 3. The description of relaxation time $\tau_{\nu\sigma}$ in the monoatomic Fe layer ν ($\nu \in 1, 6$) in the system (6Fe|3Cr|6Fe). The spacer thickness equals 4.33 Å

The effective mass dependence on the number of ferromagnetic layers was presented in [6]. The effective mass in the ultrathin films calculated by the *ab initio*

method depends also on the spin orientation and tends to $4m_e$ (m_e – the rest mass of electron) when the spins up are considered while it is limited by $5.2m_e$ when the spins down are taken into account. It is worthwhile to notice that here the conventional approach considered in various papers [1, 6] leads to an effective mass independent of approximated spin and usually it is by the value $4m_e$ for both spin orientations.

Taking into account the presented results, the giant magnetoresistance can be then calculated as

$$MR = \frac{\sigma_{\uparrow\uparrow} - \sigma_{\uparrow\downarrow}}{\sigma_{\uparrow\uparrow}} \quad (4)$$

where $\sigma_{\uparrow\downarrow}(\nu)$ and $\sigma_{\uparrow\uparrow}(\nu)$ stand for the conductivities in the case of parallel or anti-parallel magnetization between the ferromagnetic films, respectively. Each configuration results from the summation over two channels for electrons with two spin orientations [1, 6]. The contributions to GMR introduced by the surfaces, interfaces and inner monoatomic layers are shown in Fig. 4.

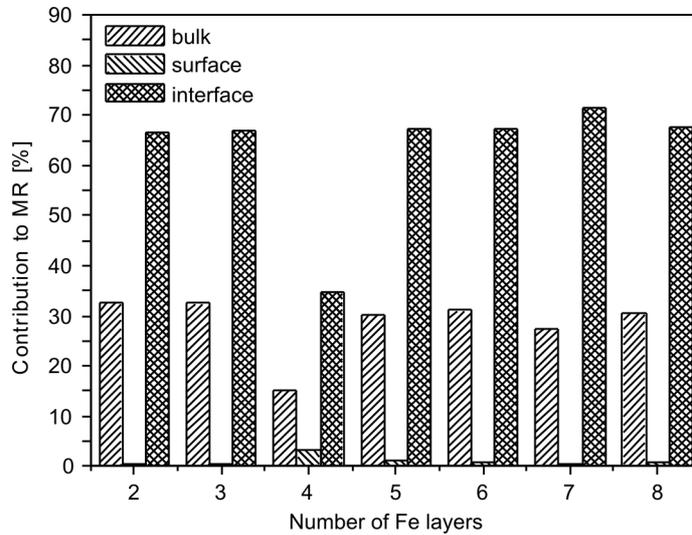


Fig. 4. Contribution to the GMR from surface, interface and inner layer position in function of the number of the ferromagnetic layer n

We can see that the contribution coming from the surface is lesser than the contribution from the interfaces which is evidently a significant part of GMR. This behaviour of the surface contribution to GMR is due to the fact that the electronic current in the plane of the surface is small and the interpretation of this fact is two-fold. On one side, a small number of electrons is localized at the surface and on the other side a large reflection of electrons from the surface barrier towards the middle layers takes its place. Both the phenomena lead to the same interpretation with respect to the number of particles while the velocity seems to be excluded as a mechanism of the surface conductivity.

4. Conclusions

First of all, our calculations show that the influence of the surface on the GMR is small when compared with the average value per monoatomic layer in the case of the system which we consider here. In contrast, the influence of the interface on GMR is evidently significant, twice greater when compared with the average value of GMR inside the sample. In this context our results confirm the experimental observations [7] and by this fact they reflect an important role of the interface behaviour for GMR description which is known in literature (e.g., [1, 5, 8]). The mechanism now established is connected with the interface potential for the electron spin dependent scattering. The bulk scattering is taken into account by introducing the spin dependent relaxation times in each monoatomic layer. In the case of semiclassical models, the number of parameters becomes so high that the formulas can only be used for a quantitative interpretation. The parameters like the relaxation time, the effective mass and the values of the potential barrier are frequently used in the literature. Nobody gives, however, numerical estimation of these parameters despite the fact that they play an important role in GMR evaluation.

Using the results obtained from DFT, we estimate the parameters which we introduce in the considerations. Thus, we estimate the contributions to GMR from the surfaces and interface layers. We can also conclude that the local values of the potential barriers depend not only on the local position of a layer (ν dependence) but also on the thickness of the total film (n dependence).

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Received 7 May 2007

Revised 21 September 2007