Origin of Giant Magnetoresistance: Bulk or Interface Scattering

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(Received 12 September 1997)

Calculations of giant magnetoresistance (GMR) of Co/Cu (001) multilayers are presented. Starting from density functional theory the electronic structure of the multilayer is described by means of a new Green's function method. Scattering of superlattice wave functions at δ-like scatterers is considered. It will be shown that due to the existence of quantum well and interface states in multilayers GMR is strongly affected by scattering centers at the interface. Results for a multilayer with a Cu thickness corresponding to the first antiferromagnetic maximum of the interlayer exchange coupling are discussed in detail. [S0031-9007(98)06042-6]

PACS numbers: 75.70.Pa, 71.20.–b, 72.15.Gd, 75.70.Cn

The discovery of giant magnetoresistance (GMR) in magnetic multilayer systems [1,2] initiated a variety of experimental and theoretical investigations to elucidate the microscopic origin of the phenomenon. It was shown by several authors [3–6] that GMR in magnetic multilayers is strongly influenced by the electronic structure of the system as a function of the magnetic configuration and it is the difference in Fermi velocities of the multilayers for parallel or antiparallel alignment of magnetic moments in adjacent magnetic layers that establishes GMR by themselves. Since this effect is a result of Bragg reflection in ideal multilayers it might be less important in dirty samples which still have a remarkable GMR amplitude. Consequently, spin-dependent scattering [7–12] is assumed to play a crucial role for GMR. Although this fact was accepted generally the question is still open if bulk or interface scattering dominates the effect. Experiments [13] and theoretical calculations [14] tended to favor interface scattering. But a microscopic explanation is missing. In this paper we present a systematic analysis of impurity scattering cross sections focusing on the peculiarities of superlattice wave functions. It will be shown that the cross sections and consequently GMR depend strongly on the position of the scatterer. To the best of our knowledge, the importance of interface states in magnetic multilayers was not realized previously.

Magnetic multilayers which display GMR are characterized by a strong potential mismatch in one spin channel which leads to the formation of quantum well and interface states. The importance of selected quantum well states for interlayer exchange coupling (IEC) was discussed already by several authors [15,16]. Moreover, it was shown [17,18] that quantum well states play a role for GMR. In this paper we demonstrate that quantum well states and especially the formation of interface states in magnetic multilayers give rise to strong interface scattering which leads to large GMR amplitudes.

All calculations are performed within the framework of density functional theory in local spin density approximation using a new Green's function method, the so-called TB KKR (tight binding Korringa-Kohn-Rostoker) [19,20]. The method is extremely advantageous for calculating the electronic structure of magnetic multilayers due to linear scaling of the numerical effort with the number N of atoms in the supercell. Furthermore, by using this method we are in position to calculate IEC and GMR on the same footing.

Since GMR occurs for systems with a magnetic ground state characterized by antiparallel orientation of the magnetic moments in adjacent magnetic layers the IEC was calculated by comparing the total energies of the system for parallel (P) and antiparallel (AP) configuration of the layer moments. Accordingly, we have chosen a multilayer geometry in the so-called first antiferromagnetic maximum of IEC consisting of 9 monolayers (ML) of Co separated by 7 ML of Cu in the (001) direction, denoted as Co_9Cu_7. The calculated antiferromagnetic maximum of 7 ML Cu is in excellent agreement with experimental results [21–23] and other calculations [24].

GMR is defined to be

$$\mathrm{GMR} = \frac{\sigma^P}{\sigma^{AP}} - 1 \tag{1}$$

with conductivities calculated within a relaxation time approximation of the transport equation for the antiferromagnetic ground state in a zero magnetic field

$$\sigma^{AP} = 2e^2 \sum_k \delta(\epsilon_k^{AP} - E_F)\tau_k^{AP}\mathbf{v}_k^{AP} \circ \mathbf{v}_k^{AP} \tag{2}$$

and for parallel alignment of the magnetic moments reached by a finite external magnetic field

$$\sigma^P = e^2 \sum_\sigma \sum_k \delta(\epsilon_k^\sigma - E_F)\tau_k^\sigma \mathbf{v}_k^\sigma \circ \mathbf{v}_k^\sigma . \tag{3}$$

Here k is a shorthand notation for the wave vector $\mathbf{k}$ and band index ν. The superscript σ indicates the

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spin direction. τ_k^σ and τ_k^{AP} denote the relaxation times characterizing the considered scattering processes for P and AP aligned moments, respectively; in general, the relaxation time is state and spin dependent. $\mathbf{v}_k^\sigma$ is the group velocity of the one-particle eigenstates (k, σ). Because of tetragonal symmetry of the supercell the conductivity in plane (CIP) is determined by the in-plane component σ_{xx} or σ_{yy} and the conductivity perpendicular to the plane (CPP) by σ_{zz}.

An important ingredient to the microscopic understanding of the conductivity is the layerwise decomposed density of states (LDOS). These local densities of states are calculated from the diagonal part of the spin-dependent one-particle Green's function of the multilayer system

$$n^\sigma(\mathbf{r}, E) = -\frac{1}{\pi} \operatorname{Im} G^\sigma(\mathbf{r}, \mathbf{r}, E)$$

$$= \sum_k |\mathring{\Psi}_k^\sigma(\mathbf{r})|^2 \delta(E - \epsilon_k^\sigma) . \qquad (4)$$

By means of the spectral representation of the Green's function they can also be resolved into a superposition of probability amplitudes of all eigenstates at energy E. The eigenstates of a supercell calculation are all Bloch states $\mathring{\Psi}_k^\sigma(\mathbf{r})$ with a normalized probability amplitude

$$\int d\mathbf{r} |\mathring{\Psi}_k^\sigma(\mathbf{r})|^2 = 1 . \qquad (5)$$

Since the conductivity is determined by electrons at the Fermi level E_F our interest is focused on LDOS and eigenstates at E_F. Consequently, the explicit energy dependence is dropped. The LDOS at E_F of the P configuration is shown in Fig. 1(a). The local density of states in the majority channel is nearly the same for all monolayers (about 2 states/spin Ry). In contrast, the minority electrons are characterized by a very inhomogeneous profile. Because of the Co d states, the local density of states is much higher in Co layers (15 states/spin Ry) than in Cu layers (2 states/spin Ry). The largest values occur at Co interface layers. This is a general behavior independent of Co or Cu layer thicknesses that can be explained in terms of eigenfunctions and their localization in the superlattice.

By means of a layerwise projection of the probability amplitude $|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{layer}})|^2$ within the supercell the electron confinement can be described. The analysis leads to four typical representatives of states [Figs. 1(b)–1(e)]. We obtain extended or free electronlike states with nearly the same probability amplitude in all layers $|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{layer}})|^2 \simeq 1/N$ [Fig. 1(b)]. Other representative states are so-called quantum well states. We obtain states with a pronounced electron confinement in Co layers. All states with an averaged probability amplitude per Co layer larger than twice the Cu layer value $[|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{Co}})|^2 > 2|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{Cu}})|^2]$ will be considered as Co quantum well states [Fig. 1(c)]. For Cu quantum well states the opposite condition has to be fulfilled $[|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{Cu}})|^2 > 2|\mathring{\Psi}_k^\sigma[\mathbf{r}_{\text{Co}})|^2]$ [Fig. 1(d)]. The most surprising states are shown in Fig. 1(e). These

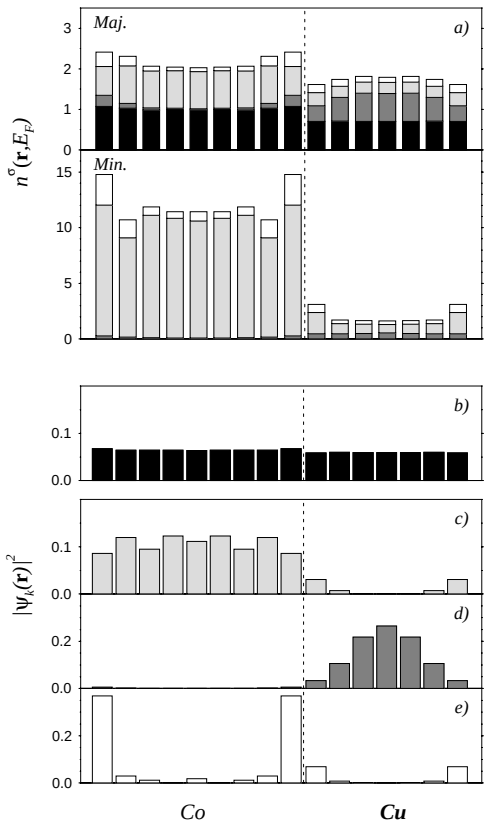

FIG. 1. Co_9Cu_7 in P configuration: Local density of states at E_F in (states/spin Ry) (a). The different shaded areas correspond to the weights of the four types of eigenstates. Probability amplitudes of representative extended (majority) (b), Co quantum well (minority) (c), Cu quantum well (minority) (d), and interface (minority) states (e) for suitably chosen **k** values.

states are characterized by a high probability amplitude at the Co interface layer. Some of these states are real interface states with an exponential decay into Co and Cu layers. But also quasilocalized states, i.e., resonances, with a high probability amplitude at the Co interface and finite but small probability amplitudes at the central layers are found. For simplicity all states with a probability amplitude $|\mathring{\Psi}_k^\sigma(\mathbf{r}_{\text{Co,inter}})|^2 > 2/N$ at the Co interface and small probability amplitudes at the central layer will be called interface states. The interface states can be understood in terms of resonance scattering and compare to the virtual bound state of a Co impurity in a Cu matrix [25]. The special shape of the probability amplitude of these states as calculated is a result of the multilayer potential and could not be obtained in a Kronig-Penney model calculation.

The spectral weight of these four types of eigenstates is indicated by the corresponding colors in Fig. 1(a). Although the classification of the eigenstates in Fig. 1(a) is arbitrary the picture is not drastically changed by modified classification conditions. Because of a smooth potential profile most of the eigenstates in the majority band are extended or free electronlike. But also Co and

Cu quantum well states and interface states appear. In contrast, the minority electrons move in a strongly varying potential with a periodicity perpendicular to the layers (z direction). For this reason all states are confined in the z direction but extended in plane. The LDOS is dominated by Co quantum well states. As can be seen from the decomposition the high LDOS at the Co interface layer is caused by Co quantum well states and interface states. These states, as will be shown later, are extremely important for GMR since they undergo a strong scattering from defects at the interface.

In the AP configuration both spin channels are dominated by quantum well states. On average, these states are less extended than states in the majority band and less localized as in the minority band.

The confinement of eigenstates is directly related to the Fermi velocities and this shows up in the conductivities. The analysis of realistic wave functions leads to the following conclusions: In general, extended states behave free electronlike with nearly the same averaged velocities in plane and perpendicular to the plane. The averaged in-plane velocity of quantum well and interface states is also of the same order of magnitude as for extended states whereas the velocity perpendicular to the planes is drastically reduced. Consequently, the quantum well states and interface states contribute mainly to CIP conductivity and give a small contribution to CPP conductivity. Since extended states dominate for the majority channel in P configuration, CIP and CPP conductivity are nearly of the same order. The minority channel is dominated by quantum well states which gives rise to a large CIP conductivity but a strongly reduced CPP conductivity. For the same reason CPP conductivity is reduced in the AP configuration since quantum well states prevent conduction. CIP conductivity in AP configuration is less influenced since quantum well states have a considerable in-plane velocity.

Because of potential scattering the transition probability is given by

$$P^{\sigma}_{kk'}(\mathbf{r}_i) = 2\pi c |T^{\sigma}_{kk'}(\mathbf{r}_i)|^2 \delta(\epsilon^{\sigma}_k - \epsilon^{\sigma}_{k'}) \qquad (6)$$

in the case of low impurity concentration c. This expression describes the scattering probability caused by an impurity at a lattice site $\mathbf{r}_i$ with respect to the supercell. The accompanying transition matrix $T^{\sigma}_{kk'}(\mathbf{r}_i)$ is defined by

$$T^{\sigma}_{kk'}(\mathbf{r}_i) = \langle \mathring{\Psi}^{\sigma}_k | \Delta V^{\sigma}(\mathbf{r}_i) | \Psi^{\sigma}_{k'} \rangle . \qquad (7)$$

$\Delta V^{\sigma}(\mathbf{r}_i)$ denotes the perturbation of the potential at the impurity site. $\mathring{\Psi}^{\sigma}_k$ and $\Psi^{\sigma}_{k'}$ are the spin-dependent unperturbed and perturbed Bloch states of the system, respectively. Since our calculations are performed at $T = 0$ spin-flip scattering is neglected. The relaxation time is then given by

$$[\tau^{\sigma}_k(\mathbf{r}_i)]^{-1} = \sum_{k'} P^{\sigma}_{kk'}(\mathbf{r}_i) . \qquad (8)$$

To focus on the influence of the superlattice wave functions to the relaxation time we neglect details of the impurity potential and assume a δ scatterer with the same spin-dependent scattering strength t^{σ} at all lattice sites

$$\Delta V^{\sigma}(\mathbf{r}_i) = t^{\sigma} \delta(\mathbf{r} - \mathbf{r}_i) \qquad (9)$$

with a spin anisotropy ratio $\beta = (t^{\downarrow}/t^{\uparrow})^2$. Consequently, the spin-dependent relaxation time in Born approximation becomes

$$[\tau^{\sigma}_k(\mathbf{r}_i)]^{-1} = 2\pi c |\mathring{\Psi}^{\sigma}_k(\mathbf{r}_i)|^2 n^{\sigma}(\mathbf{r}_i, E_F) t^{\sigma 2} + \tau^{-1} . \qquad (10)$$

To avoid short circuit effects due to states with a tiny probability amplitude at the impurity position a constant and spin-independent inverse relaxation time τ^{-1} is added. The amount of τ^{-1} is chosen to be on average of the same order as the first term of Eq. (10).

The result of Eq. (10) can also be interpreted in terms of multiple scattering theory and would correspond to a single site approximation neglecting all backscattering effects. t^{σ} would then be the difference of single site transition matrices of impurity and host.

Since the relaxation time [Eq. (10)] is proportional to the spin dependent LDOS at the impurity site $n^{\sigma}(\mathbf{r}_i, E_F)$ we expect a strong position dependence. Because of the large enhancement of LDOS at the Co interface layer [Fig. 1(a)] impurities in this position will be the most effective scatterers in comparison to all other positions. Furthermore, from the knowledge of spectral weights and probability amplitudes it is clear that at the interface position Co quantum well states and interface states are strongly scattered.

The influence of the position dependent impurity scattering cross sections to GMR is shown in Fig. 2. The case of vanishing t^{σ} describes the scattering at homogenously distributed defects causing an averaged spin-independent relaxation time τ [see Eq. (10)] which leads to straight lines at 30% for CIP-GMR and 125% for CPP-GMR.

The triangles show GMR results for one impurity with no spin anisotropy ($\beta = 1$) at all possible positions in the supercell. As expected, the GMR amplitude is strongly enhanced by defects at the Co interface layer and slightly

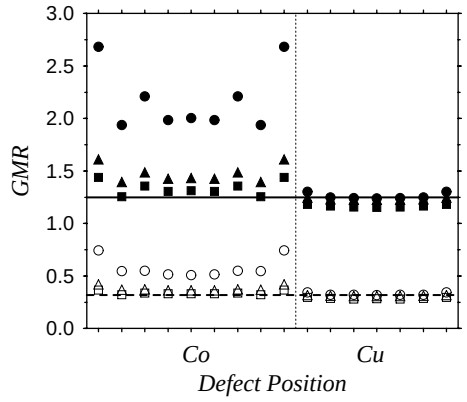

FIG. 2. GMR of Co_9Cu_7: open symbols for CIP-GMR, closed symbols for CPP-GMR; $t^{\sigma} = 0$, dashed and full lines; $\beta = 0.25$, squares; $\beta = 1.0$, triangles; $\beta = 4.0$, circles.

enhanced by bulk defects in Co. Defects in Cu are absolutely ineffective for GMR which is related to the small LDOS in Cu [see Fig. 1(a)].

With spin-dependent scattering $\beta > 1$, that is, stronger scattering of minority than majority electrons, the existing spin anisotropy of LDOS is amplified and leads to an even stronger enhancement of the GMR amplitudes. For opposite spin anisotropy $\beta < 1$ the spin anisotropy of LDOS and scattering potential compensate each other and GMR is reduced in comparison to the spin-independent case. The above discussed position dependence is, of course, reflected in both cases. It is well known from residual resistivities of dilute alloys [27] that, depending on the valence difference between impurity atom and host, spin anisotropies β smaller or larger than 1 can be obtained for one and the same host. In particular, Cu impurities in bulk Co or Ni have anisotropies $\beta = 1.85$ [26] and $\beta = 3.7$ [27], respectively.

In conclusion, we have shown using wave functions of a periodic multilayer that quantum well and interface states give large contributions mainly to CIP conductivity whereas CPP conductivity is caused by extended states. Furthermore, our results demonstrate that, due to quantum well and interface states, the GMR amplitude depends strongly on the position of the scatterers and favors interface scattering in agreement with experiments [13]. The calculations suggest that smooth interfaces with impurities in the Co layer and with large β values ($\beta > 1$) lead to high GMR amplitudes in Co/Cu multilayers.

One of us (I. M.) thanks P. M. Levy and A. Fert for helpful discussions. This work was partly supported by the BMBF Contract No. 05 621 ODA 7 and NATO Grant No. CRG 960340.

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