AB-INITIO THEORY OF THE CPP-MAGNETOCONDUCTANCE *)

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The current-perpendicular-to-plane (CPP) magnetoconductance of a trilayer consisting of a spacer sandwiched between two ideal leads is described on an *ab initio* level. We employ the transmission matrix formulation of the conductance within the framework of the spin-polarized surface Green function technique as formulated in terms of the tight-binding linear muffin-tin orbital method. The formalism is extended to the case of lateral supercells in each layer with random arrangements of atoms which allows to treat both the ballistic and diffusive transports on equal footing. The application is made to fcc-based Co/Cu/Co(001) trilayers.

I Introduction

Transport in layered materials has been a subject of intensive theoretical investigations, in particular in view of the discovery of the giant magnetoconductance (GMC) in metallic multilayers [1]. Most of measurements up to date were reported for the current-in-plane (CIP) geometry [2] since the current-perpendicular-to-plane (CPP) geometry [3] is experimentally more challenging. The CPP transport is also closely related to the tunneling through non-metal and to the ballistic transport [4].

Ab initio calculations of the GMC are still rather rare. We mention the method of Boltzmann-equation applied to multilayers [5] and a Kubo-Greenwood approach generalized to layered systems in terms of the layered Korringa-Kohn-Rostoker (KKR) method [6] and the relativistic spin-polarized screened KKR method [7] but neglecting the so-called coherent CPA (coherent potential approximation) vertex corrections. Both approaches can be used for the CIP and CPP regimes.

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Alternative theoretical approaches applicable to the CPP transport are based either on the non-equilibrium Green function method [8] or on a transmission matrix formalism [9] and were implemented within an empirical tight-binding (TB) method. These methods are based on the formalism of the surface Green functions (SGF) and their numerical requirements scale linearly with the system size.

It is the aim of this paper to formulate such approach within the first principles tight-binding linear-muffin orbital (TB-LMTO) method and for a general stacking of non-random layers (ballistic transport). This formulation will be then extended to the case of two-dimensional supercells in each layer with a random occupation of lattice sites. The usefulness of such approach has recently been illustrated for the case of a single-band TB model [10]. An application is made to the case of Co/Cu/Co(001)-based trilayers.

II Formalism

We wish to determine the conductance of a system which consists of a semi-infinite left ($\mathcal{L}$) and a right ($\mathcal{R}$) magnetic lead sandwiching a non-magnetic spacer of varying thickness. Both the spacer and/or interfaces between the magnetic leads and the spacer can in principle be random (a substitutional binary alloy). The sequence of layers in the growth direction of the trilayer is assumed to be arbitrary, and each layer can be partitioned into supercells containing $n \times n$ lattice sites occupied at random by two atom species. We neglect possible layer and lattice relaxations in the system.

A Electronic structure

The electronic structure of the system is described by the TB-LMTO Hamiltonian,

$$H^{\gamma,\sigma}_{\mathbf{R}L,\mathbf{R}'L'} = C^{\sigma}_{\mathbf{R}L}\,\delta_{\mathbf{R},R'}\delta_{L,L'} + (\Delta^{\sigma}_{\mathbf{R}L})^{1/2}\,\left\{S^{\beta}\,\left(1-(\gamma-\beta)\,S^{\beta}\right)^{-1}\right\}_{\mathbf{R}L,\mathbf{R}'L'}\,(\Delta^{\sigma}_{\mathbf{R}'L'})^{1/2}\,. \quad (1)$$

Here, $\mathbf{R}$ is the site index, σ is the spin index, the potential parameters $C^{\sigma}_{\mathbf{R}}$, $\Delta^{\sigma}_{\mathbf{R}}$, and $\gamma^{\sigma}_{\mathbf{R}}$ are diagonal matrices with respect to the orbital index $L = (\ell m)$, the non-random screened structure constants matrix $S^{\beta}_{\mathbf{R}L,\mathbf{R}'L'}$ is spin-independent, and $\beta_{\mathbf{R},LL'} = \beta_L\,\delta_{L,L'}$ is the screening matrix. Assuming one and the same two-dimensional translational symmetry in each layer n, $\mathbf{k}_{\parallel}$-projections can be defined, where $\mathbf{k}_{\parallel}$ is a vector from the corresponding surface Brillouin zone (SBZ). In a principal layer formalism [11], the screened structure constants $S^{\beta}_{p,q}$ are of block tridiagonal form,

$$S^{\beta}_{p,p}(\mathbf{k}_{\parallel}) = S^{\beta}_{0,0}(\mathbf{k}_{\parallel}),\quad S^{\beta}_{p,q}(\mathbf{k}_{\parallel}) = S^{\beta}_{0,1}(\mathbf{k}_{\parallel})\,\delta_{p+1,q} + S^{\beta}_{1,0}(\mathbf{k}_{\parallel})\,\delta_{p-1,q}\,. \quad (2)$$

The properties of individual atoms occupying lattice sites are characterized by potential function matrices,

$$P_{\mathrm{R}}^{\beta,\sigma}(z) = \frac{z - C_{\mathrm{R}}^{\sigma}}{\Delta_{\mathrm{R}}^{\sigma} + (\gamma_{\mathrm{R}}^{\sigma} - \beta)\,(z - C_{\mathrm{R}}^{\sigma})}\,, \tag{3}$$

which are diagonal with respect to L and obtained by solving the corresponding Schrödinger equation within the density functional formalism. In a case of binary substitutional alloy the potential functions assume two different values to be determined within the CPA. Finally, we define the Green function matrix $g^{\beta,\sigma}(z)$ in the TB-LMTO method as

$$\left(g^{\beta,\sigma}(\mathbf{k}_{\parallel}, z)\right)^{-1}_{p,q} = P_{p}^{\beta,\sigma}(z)\,\delta_{p,q} - S_{p,q}^{\beta}(\mathbf{k}_{\parallel})\,. \tag{4}$$

We refer the reader to a recent book [11] for further details concerning the TB-LMTO method for disordered layered systems.

B Magnetoconductance

Our derivation of the magnetoconductance C follows that given in [8] and its details will be published elsewhere. The resulting expression is

$$C = \sum_{\sigma} C^{\sigma}\,, \quad C^{\sigma} = \frac{e^2}{h}\,\frac{1}{N_{\parallel}} \sum_{\mathbf{k}_{\parallel}} T^{\sigma}(\mathbf{k}_{\parallel}, E_{\mathrm{F}})\,, \tag{5}$$

where $N_{\parallel}$ is the number of $\mathbf{k}_{\parallel}$ in the SBZ and E_{F} is the system Fermi energy. The transmission coefficient $T^{\sigma}(\mathbf{k}_{\parallel}, E)$ is given by

$$T^{\sigma}(\mathbf{k}_{\parallel}, E) = \mathrm{tr}\left\{B_{1}^{\beta,\sigma}(\mathbf{k}_{\parallel}, E)\, g_{1,N}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{+})\, B_{N}^{\beta,\sigma}(\mathbf{k}_{\parallel}, E)\, g_{N,1}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{-})\right\}, \tag{6}$$

where tr denotes the trace over the orbital index L,

$$\begin{aligned} B_{1}^{\beta,\sigma}(E) &= \mathrm{i}\,S_{1,0}^{\beta}(\mathbf{k}_{\parallel})\,\left[\mathcal{G}_{\mathcal{L}}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{+}) - \mathcal{G}_{\mathcal{L}}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{-})\right]\, S_{0,1}^{\beta}(\mathbf{k}_{\parallel})\,, \\ B_{N}^{\beta,\sigma}(E) &= \mathrm{i}\,S_{0,1}^{\beta}(\mathbf{k}_{\parallel})\,\left[\mathcal{G}_{\mathcal{R}}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{+}) - \mathcal{G}_{\mathcal{R}}^{\beta,\sigma}(\mathbf{k}_{\parallel}, z_{-})\right]\, S_{1,0}^{\beta}(\mathbf{k}_{\parallel})\,, \end{aligned} \tag{7}$$

and $z_{\pm} = E \pm \mathrm{i}\delta$. The quantities $\mathcal{G}_{\mathcal{X}}^{\beta,\sigma}$, $\mathcal{X} = \mathcal{L}, \mathcal{R}$ are the SGFs of the ideal left and right leads [11], respectively. The magnetoconductance ratio is defined as $R_{\mathrm{GMC}} = -1 + C_{\mathrm{F}}/C_{\mathrm{AF}}$, where F (AF) denote the ferromagnetic (antiferromagnetic) configurations of magnetizations in the leads, respectively.

A generalization of the formalism to the case of two-dimensional supercells is straightforward as the equations remain formally identical, only the matrices are replaced by supermatrices with respect to inequivalent atoms in the supercell.

III Results and discussion

We have performed calculations for three geometries:

(i) ideal Co/Cu interfaces (the ballistic case),

(ii) interdiffused interfaces (two neighboring interface layers are disordered with compositions $Co_{85}Cu_{15}$ and $Co_{15}Cu_{85}$), and

(iii) random $Cu_{85}Ni_{15}$ spacer sandwiched by pure Co assuming an fcc(001) stacking of layers.

Single-band TB calculations ($n \times n$-supercells, $n = 5$, 7, and 10) have confirmed that already 5×5-supercells can give quite representative results. The same random 5×5-supercells (21 A-atoms and 4 B-atoms) averaged over 5 different configurations were also used in the TB-LMTO calculations. The input potential functions were

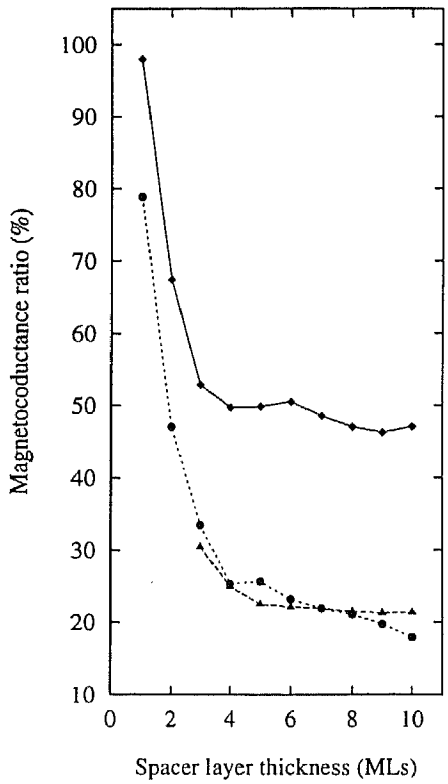

Fig. 1. Magnetoconductance ratio for the ideal Co/Cu/Co trilayer (ballistic limit, diamonds), for the Co/Cu/Co trilayer with interdiffused interfaces (triangles), and for the $Co/Cu_{85}Ni_{15}/Co$ trilayer with a random spacer (bullets).

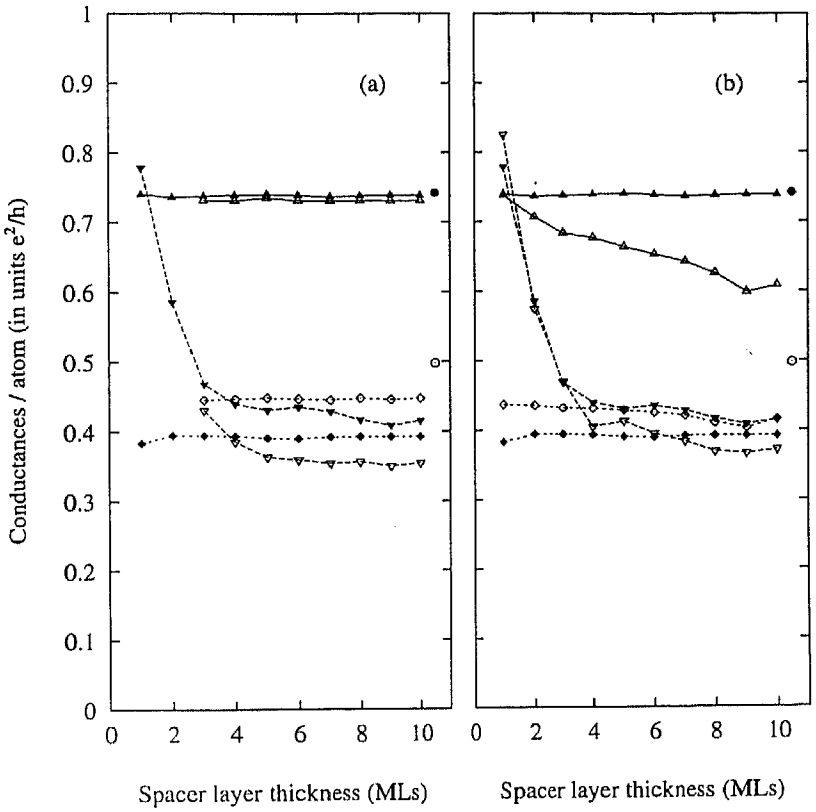

Fig. 2. Conductances per atom for the ferromagnetic configuration (↑-spin, triangles, and ↓-spin, inverted triangles) and for the antiferromagnetic configuration (diamonds, the same for ↑- and ↓-spins) for (a) the Co/Cu/Co trilayer with interdiffused interfaces, and (b) for the $Co/Cu_{85}Ni_{15}/Co$ trilayer with a random spacer (empty symbols). The results for the ideal Co/Cu/Co trilayer are given by full symbols. Conductances for a single Co/Cu(001) interface (↑-spin, bullet, and ↓-spin, circle) are also given for reference.

determined selfconsistently for a given alloy composition using the CPA [11] and it was verified that possible current fluctuations due to different supercells are small. The $\mathbf{k}_\parallel$-integration extends over 10000 points in the full fcc(001)-SBZ (400 points in the corresponding supercell SBZ) and $|\mathrm{Im}\, z_\pm| = 10^{-7}$ Ry.

The GMC ratio is plotted in Fig. 1, whereas the F and AF conductances for ↑- and ↓ -spin electrons are plotted in Fig. 2 as a function of the spacer thickness. It should be noted that for a symmetric geometry as used in here the AF-↑ and AF-↓ conductances are identical. In the interdiffused case, the first unperturbed spacer layer corresponds to the third layer of the ideal interface, etc. The following conclusions can be made:

(i) The quantum oscillations of the GMC in the ballistic limit (see also Mathon [9]) are due to multiple scatterings of primary ↓-spin electrons at the system interfaces. They are damped with increasing spacer thickness (not shown here) reaching a limit of about 50%;

(ii) Disorder generally suppresses the GMC. For the case of mixed interfaces the above-mentioned quantum oscillations are strongly suppressed and the GMC quickly reaches its saturation value of about 20%. In the case of a random spacer we observe a pronounced thickness dependence of the GMC ratio which seems to saturate at a value slightly below 20%;

(iii) The F↑-conductances are nearly the same in the ballistic case and in the case of mixed interfaces because of the similarity of the Cu- and the Co ↑-bands at the Fermi energy. They are also quite close to the reference conductance of a single CoCu-interface. The F↑-conductance for random spacer differs from that in the ballistic case: the Ni- and Co ↑-bands are now different;

(iv) The F↓-conductance in the ballistic limit approaches that of a single CoCu-interface, but remains somewhat smaller (effect of multiple scatterings at two interfaces). In disordered cases the F↓-conductances are smaller than in the ballistic limit. The strong disorder of the Cu- and the Co ↓ states is the reason for a suppression of quantum oscillations mentioned above. On the other hand, disorder in the spacer influences the F↓-conductance only weakly: the dependence of the conductance on the spacer thickness follows closely that found in the ballistic case and it is only slightly reduced as the effect of disorder in Cu-rich CuNi alloy is rather weak at the Fermi energy;

(v) Finally, the AF↑- and AF↓-conductances are in all cases nearly independent of the spacer thickness reaching quickly their saturation values which are close to that of the F↓-conductance. It should be noted that the AF-conductance in the ballistic case is slightly smaller as compared to the disordered cases. This is a result of competition between bandstructure effects and the influence of disorder: both Ni-impurities in Cu and Cu-impurities in Co lower average potential barrier seen by ↓-spin electrons.

The supercell calculations are in principle exact and we have compared them with the CPA transport calculations neglecting vertex corrections ($g^{\sigma}(z)$ in Eq. (6) are averaged independently using the CPA). The results gave too small conductances indicating the necessity of including vertex corrections in the case of the CPP transport.

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