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Spin-Mixing Conductances of Ni-Based Films Attached to Cu(100) Leads

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The complex spin-mixing conductance of epitaxial Cu/Ni/Cu(100) systems is predicted to oscillate as a function of Ni thickness. The oscillation period is explained in terms of spin-resolved Fermi surface properties of bulk nickel. Stability of the oscillations with respect to interface Cu–Ni interdiffusion and to alloying in the Ni film is investigated as well.

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1. Introduction

Spin-mixing conductance of an interface between a non-magnetic metal and a ferromagnet represents an important concept in non-collinear magnetoelectronics [1, 2]. This complex quantity provides — together with the usual spin-resolved conductances in current-perpendicular-to-plane (CPP) geometry — complete information on a linear response of particle and spin currents due to the bias and spin accumulation in the adjacent metals. Recent *ab initio* studies of the spin-mixing conductance for thin ferromagnetic films (Fe, Co) attached to two non-magnetic metallic leads (Cu, Au, Cr) [2, 3] have proved that this quantity saturates very rapidly with increasing film thickness. This behavior is equivalent to a very short magnetic coherence length due to large differences between the majority and minority Fermi surfaces of the bulk ferromagnet [2]. However, this may not hold for Ni-based systems with a weak exchange splitting. The present paper is thus devoted to Ni(100) films with a face-centered cubic (fcc) structure epitaxially embedded between two fcc Cu(100) leads.

2. Theory and implementation

The spin-mixing conductance per unit two-dimensional (2D) cell of the magnetic film is within the tight-binding linear muffin-tin orbital method [4] given

explicitly by [5]:

$$C_{\mathcal{L}}^{\mathrm{mix}} = \frac{e^2}{h}\frac{1}{N_{\parallel}}\mathrm{Tr}\left[\mathrm{i}\left(g_{\uparrow}^{\mathrm{r}} - g_{\downarrow}^{\mathrm{a}}\right)\mathcal{B}_{\mathcal{L}} - \left(\mathcal{B}_{\mathcal{L}} + \mathcal{B}_{\mathcal{R}}\right) g_{\uparrow}^{\mathrm{r}} \mathcal{B}_{\mathcal{L}} g_{\downarrow}^{\mathrm{a}}\right], \tag{1}$$

where $N_{\parallel}$ denotes a large number of 2D cells in directions parallel to atomic layers and the trace refers to orbitals of an intermediate region comprising the magnetic film and a few neighboring atomic layers of the non-magnetic leads. The quantities g_s^{r} and g_s^{a} ($s = \uparrow, \downarrow$) denote spin-resolved auxiliary Green's-function matrices calculated respectively at energies $E_{\mathrm{F}} + \mathrm{i}\eta$ and $E_{\mathrm{F}} - \mathrm{i}\eta$, where E_{F} denotes the Fermi energy and $\eta \to 0^+$. The spin-independent matrices $\mathcal{B}_{\mathcal{L}}$ and $\mathcal{B}_{\mathcal{R}}$ correspond to anti-Hermitian parts of self-energies of the left ($\mathcal{L}$) and the right ($\mathcal{R}$) leads [6].

The calculations of underlying self-consistent electronic structures, the treatment of substitutional randomness in the films, and the computational details were described elsewhere [5, 6].

3. Results and discussion

The spin-resolved CPP conductances of the Cu/Ni/Cu(100) system with ideal (sharp) interfaces depend only negligibly on Ni thickness, whereas the spin--mixing conductance is characterized by pronounced oscillations with a period of 11 monolayers (ML) and with a large amplitude slowly decaying with increasing Ni thickness, see Fig. 1. The origin of these oscillations has to be identified with stationary points of the difference $k_{i\perp}^{\uparrow} - k_{j\perp}^{\downarrow}$ as a function of the $\boldsymbol{k}_{\parallel}$ vector in the (100) plane where i and j run over individual sheets of the bulk fcc Ni Fermi surface in the two spin channels [2, 3].

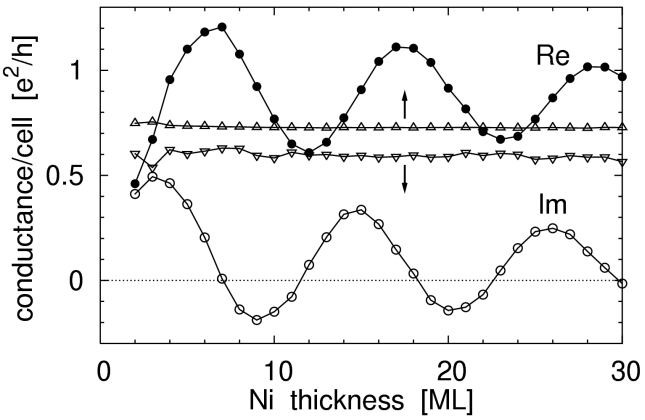

Fig. 1. The CPP conductances of Cu/Ni/Cu(100) as functions of the Ni thickness: spin-resolved conductances for majority (↑) and minority (↓) electrons and the real (Re) and the imaginary (Im) parts of the complex spin-mixing conductance.

Cross-sections of the majority $e_6^{\uparrow}$ and the minority $e_6^{\downarrow}$ sheets [7] in the plane (001) are shown in Fig. 2; they give rise to a stationary point of the difference

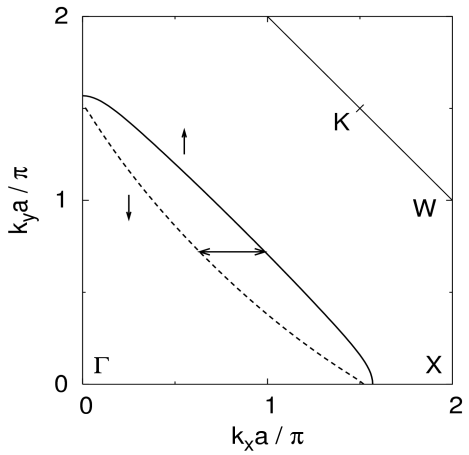

Fig. 2. Cross-section of the Ni Fermi surfaces for majority (↑, full curve) and minority (↓, dashed curve) spin channels in the (001) plane. The horizontal arrow denotes the position of the $\boldsymbol{k}_{\parallel}$ vector in the (100) plane corresponding to the stationary point of the difference $k_{\perp}^{\uparrow} - k_{\perp}^{\downarrow}$. The labels Γ, X, W, and K refer to special points of the fcc Brillouin zone.

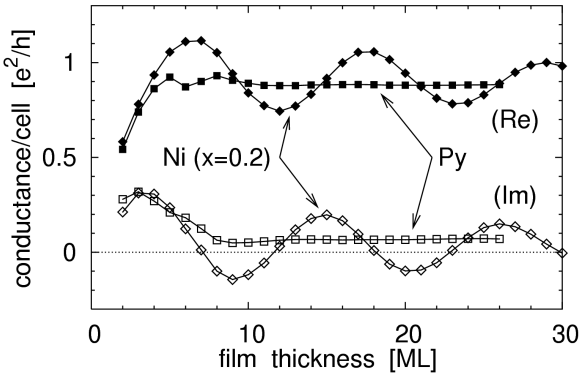

Fig. 3. The spin-mixing conductances of Cu/Py/Cu(100) and of Cu/Ni/Cu(100) with interdiffused interfaces ($x = 0.2$) as functions of the magnetic film thickness.

$k_{\perp}^{\uparrow} - k_{\perp}^{\downarrow}$. The resulting stationary value $\Delta k_{\perp} \approx 1.111 a^{-1}$, where a is the fcc lattice parameter, yields oscillations with a period $\Lambda = 2\pi/\Delta k_{\perp} \approx 11.3$ ML, in a very good agreement with the data in Fig. 1.

The spin-mixing conductances of the Cu/Py/Cu(100) system (where Py denotes a random fcc $Ni_{0.84}Fe_{0.16}$ alloy) and of the Cu/Ni/Cu(100) system with interdiffused interfaces (simulated by random 2D alloys of compositions $Cu_{1-x}Ni_x$ and Cu_xNi_{1-x} with $x = 0.2$ in two atomic layers at the interfaces) are plotted in Fig. 3. One can see that Fe impurities are very efficient in suppressing the oscillations found for pure Ni films. On the other hand, the oscillations are rea-

sonably stable with respect to interface interdiffusion, which makes the studied Cu/Ni/Cu(100) system suitable for possible experimental verification of the predicted oscillatory behavior.

Acknowledgments

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