2004

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Journal of Magnetism and Magnetic Materials 272–276 (2004) 1954–1955
journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Spin-dependent tunneling from clean and oxidized Co surfaces

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Abstract

Transmission through a sufficiently thick vacuum barrier is factorized in the product of two "surface transmission functions" and a vacuum decay factor. Based on this factorization, we study the spin polarization of the tunneling current from clean and oxidized (1 1 1) FCC Co surfaces through vacuum into Al. The conductance is calculated using the principal-layer Green's function approach within the tight-binding LMTO scheme. We find that for typical vacuum barrier thicknesses the tunneling current from the clean surface is dominated by minority-spin electrons. A monolayer of oxygen on top of the surface completely changes the shape of $\mathbf{k}_{\parallel}$-resolved transmission and makes the tunneling current almost 100% majority-spin polarized.

PACS: 72.25.Mk; 73.40.Gk; 73.40.Rw; 73.23.−b

Keywords: Spin-dependent tunneling; Principal-layer Green's function approach; Magnetic tunnel junction

Spin-dependent tunneling (SDT) in magnetic tunnel junctions is strongly affected by the atomic and electronic structure of the interfaces between the electrodes and the insulating barrier (for a review of SDT see Ref. [1]). In this paper, using vacuum as a barrier, we study the effect of surface oxidation on SDT. Representing the transmission as a product of contributions of two surfaces and the barrier, we calculate the tunneling conductance from clean and oxidized Co surfaces into Al, and show that oxidation has a dramatic effect on the spin polarization (SP) of the tunneling current.

For a thick barrier, one may approach the tunneling problem in the spirit of perturbation theory [2]. In this limit, the reflection and transmission at each interface are almost unaffected by the presence of the other one, and the eigenstates inside the barrier do not differ much from those of an infinitely thick barrier. Let us focus on the vacuum barrier and assume that translational periodicity is preserved at each surface, but it should not necessarily be the same for both. Each Bloch wave with a lateral quasi-wave vector $\mathbf{k}_{\parallel}$ from the left lead has a decay tail in the vacuum composed of the waves with lateral wave vectors $\mathbf{k}_{\parallel}+\mathbf{G}_i$, where $\mathbf{G}_i$ are the reciprocal lattice vectors of the surface Brillouin zone of the left lead [3]. At a sufficient distance from the surface (typically a few lattice parameters) all waves with $\mathbf{G}_i \neq 0$ vanish and may be neglected. This means that $\mathbf{k}_{\parallel}$ is conserved across the entire system even if there is no common in-plane periodicity. It follows that the transmission $T(\mathbf{k}_{\parallel})$ is factorized:

$$T^{\sigma}(\mathbf{k}_{\parallel}) = t^{\sigma}_{\mathrm{L}}(\mathbf{k}_{\parallel})\exp[-2\kappa(\mathbf{k}_{\parallel})d]t^{\sigma}_{\mathrm{R}}(\mathbf{k}_{\parallel}), \quad (1)$$

where we introduced the *surface transmission functions* (STF) t^{σ}_{L}, t^{σ}_{R} characterizing the left and right surfaces, and $\kappa(\mathbf{k}_{\parallel})$ is the vacuum decay parameter determined by the work function. STF is equal to the Fermi-level value of the $\mathbf{k}_{\parallel}$-resolved density of states for the given spin σ generated by the incoming Bloch states and taken at a

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doi:10.1016/j.jmmm.2003.12.499

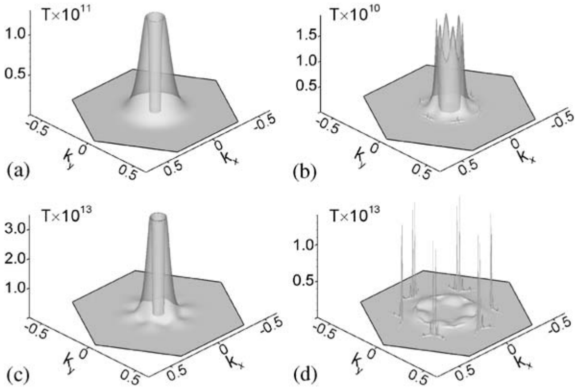

Fig. 1. $\mathbf{k}_{\|}$-resolved transmission from clean and oxidized (1 1 1) Co surfaces through vacuum into Al. (a) Clean surface, majority spin. (b) Clean surface, minority spin. (c) Oxidized surface, majority spin. (d) Oxidized surface, minority spin. The vacuum layer thickness is 2 nm for clean and 1.7 nm for oxidized Co surface. X and Y are in units of the smallest G.

certain reference distance from the surface. In Eq. (1) d is the distance between left and right reference planes.

Using Eq. (1), we calculated $T(\mathbf{k}_{\|})$ for tunneling between a (1 1 1) FCC Co lead with a clean or oxidized surface and an Al lead. This setup is relevant to experiments on spin-polarized tunneling [4], but we replace the insulating barrier by vacuum. We used the principal-layer Green's function approach [5] based on the tight-binding LMTO method and the transmission matrix formulation of Ref. [6]. All atomic potentials were determined self-consistently. The oxidized Co surface with one oxygen monolayer was fully relaxed using the pseudopotential plane-wave method [7]. The results are shown in Fig. 1. The Fermi surface (FS) of Co in the [1 1 1]-direction has holes around the $\bar{\Gamma}$ point with no bulk states in both spin channels, which results in zero conductance in this area (see Fig. 1a,b). The hole in the majority spin channel is smaller, and asymptotically, for thick barriers, the conductance becomes fully majority-spin polarized. However, this asymptotic behavior only sets in at $d \sim 10$ nm, while for barrier thicknesses $d \sim 1-2$ nm typical for SDT experiments the SP is about -60% and depends weakly on d. Minority-spin transmission (Fig. 1b) has a crown-shaped "hot spot" around the edge of the FS hole. The analysis of layer and $\mathbf{k}_{\|}$-resolved density of states (DOS) shows that it is not associated with surface states [8], but rather with an enhancement of bulk $\mathbf{k}_{\|}$-resolved DOS near the FS edge.

Oxidation of the Co surface creates a strong spin-filter effect. As it is evident from Fig. 1c, oxidation does not significantly change the shape of the $\mathbf{k}_{\|}$-resolved transmission for majority-spin electrons. On the contrary, it strongly suppresses tunneling of those minority-spin states that dominated the conductance for the clean Co surface (Fig. 1d). This reverses sign of the SP making the conductance almost 100% positively spin-polarized. This effect demonstrates the crucial role of surface atomic and electronic structure in SDT.

This work was supported by NSF (DMR-0203359 and MRSEC DMR-0213808) and the Nebraska Research Initiative.

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