Spin-Dependent Surface Screening in Ferromagnets and Magnetic Tunnel Junctions

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We have examined electron screening at the surface of a ferromagnetic metal. In an applied electric field, the surface develops an induced charge and magnetization. This can be described in terms of a novel spin-dependent screening electric field. A set of integrodifferential equations for screening potentials is derived and solved in some limiting cases. The significant implication relevant to spin-polarized transport in field emission and in magnetic tunnel junctions is discussed.

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Electron screening in the surface of a nonmagnetic metal in an externally applied field is well understood [1,2]. A dc electric field penetrates only about a Thomas-Fermi screening length into the metal. There develops a surface buildup of electric charges which screen the bulk of the metal from the applied field. For a *ferromagnetic* metal, screening charges at the surface might well influence the surface magnetization. The importance of the exchange effect on electron screening in ferromagnets has already been shown by del Moral *et al.* when they studied crystal-field magnetoelastic stress in rare-earth compounds and superlattices [3]. In this Letter, we model electric screening effects in a ferromagnet by studying the dielectric response of its surface to an applied electric field. To properly account for charge and magnetization buildup, we found it very advantageous to explicitly introduce an important new concept, which we call the spin-dependent screening potential.

The spin dependence of the screening potential originates from the exchange interaction in ferromagnets. When electron charges build up at the surface of the ferromagnet, they interact via Coulomb interactions which depend on the total net charges and via ferromagnetic exchange interactions which depend on the spin of the screening charges, i.e., the spin up and down electrons will have different potentials. These different potentials can be interpreted as voltage absorbed by the ferromagnet, or as spin-dependent electric field penetrating into the ferromagnet. We should point out here that the concept of the spin dependence of potentials introduced here is different from that of the spin accumulation in magnetic multilayers [4]. In magnetic multilayers, spin accumulation is proportional to electric current, i.e., it is a *current driven* effect. Chui has extended this current driven spin accumulation to magnetic tunnel junctions (MTJ) [5]. In the present model, we consider the spin-dependent electric field due to externally applied voltage, i.e., it is a *voltage driven* effect. In the case of infinite tunnel resistance, the spin accumulation due to the current driven effect is zero, while the voltage driven effect remains. Furthermore, the current driven spin accumulation leads to differences in chemical potentials for spin up and down electrons while the voltage driven magnetization results in spin-dependent band bendings as we will show later. We should first construct a set of general integrodifferential equations which govern the charge and magnetization buildup at the surface. The equations are then solved in some limiting cases. In particular, we estimate the induced magnetic moments by an applied electric field in Ni, Co, and Fe.

Consider an electric field applied normally to the surface defined as the $x = 0$ plane. We introduce an induced charge density $\delta n(x)$ so that the total charge density is $n(x) = n_0 + \delta n(x)$ where n_0 is the charge density in the absence of the applied field. In a ferromagnet, let this charge density be explicitly written as the sum of two spin channels, i.e., $n(x) = n^{\uparrow}(x) + n^{\downarrow}(x)$ where $n^{\sigma}(x) = n_0^{\sigma} + \delta n^{\sigma}(x)$. The induced charges interact via Coulomb interactions and give rise to a Coulomb energy,

$$W_c = \frac{e^2}{8\pi\epsilon_0}\int \frac{[\delta n^{\uparrow}(x) + \delta n^{\downarrow}(x)]\cdot[\delta n^{\uparrow}(x') + \delta n^{\downarrow}(x')]}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}'. \tag{1}$$

In a ferromagnetic metal, the induced charges are also subjected to exchange interactions. While there are numbers of forms to express the exchange interactions, we find it convenient to limit ourselves within the Stoner rigid two-spin band model, i.e., spin up and down bands are split by an exchange constant. Then the exchange energy W_e can be expressed as $W_e = (1/2)H_{\rm eff}\cdot\delta M$, where $H_{\rm eff}$ is the internal exchange field in the ferromagnet, $\delta M = (\delta n^{\uparrow} - \delta n^{\downarrow})\mu_B$ is the induced magnetic moment, and μ_B is the Bohr magneton. While the detailed determination of $H_{\rm eff}$ is difficult, it is usually parametrized as $H_{\rm eff} = JM/\mu_B^2$, where J is the order of the exchange splitting of the spin-up and spin-down bands (which have been estimated for Ni, Co, and Fe as will be discussed later), and $M = [n^{\uparrow}(x) - n^{\downarrow}(x)]\mu_B$ is the total magnetization. With this parametrization, the exchange energy is

$$W_e = (J/2)[(n_0^{\sigma} - n_0^{-\sigma})[\delta n^{\sigma}(x) - \delta n^{-\sigma}(x)] + (J/2)[\delta n^{\sigma}(x) - \delta n^{-\sigma}(x)]^2, \tag{2}$$

where σ is the spin index for the majority or minority electrons. The screening electron energy is the sum of the Coulomb term and the exchange term. We formally define a *spin-dependent* potential U^σ by taking a functional derivative of the screening electron energy with respect to $\delta n^\sigma(\mathbf{r})$,

$$eU^\sigma(x) \equiv \frac{\partial(W_c + W_e)}{\partial \delta n^\sigma(x)} = E_0^\sigma + eV_c(x) + J[\delta n^\sigma(x) - \delta n^{-\sigma}(x)], \tag{3}$$

where $V_c(x)$ satisfies Poisson's equation, i.e.,

$$\frac{d^2V_c(x)}{d^2x} = -(e/\epsilon_0)[\delta n^\uparrow(x) + \delta n^\downarrow(x)], \tag{4}$$

and $E_0^\sigma = (J/2)(n_0^\sigma - n_0^{-\sigma})$ is the exchange potential of the ferromagnet; it is independent of charge buildup and the difference of the potentials for spin up and spin down is precisely the splitting of the spin up and down bands, $J(n_0^\uparrow - n_0^\downarrow)$. The second and third terms in Eq. (3) are the potentials due to induced charges; one can interpret them as the electric field (spatial derivative of the potential) penetrating into the magnetic metal. The second term is from the Coulomb interaction among buildup charges, which is usually the focus in discussing the electron screening in metals and degenerate semiconductors. The third term, which is absent in nonmagnetic metals, appears as a consequence of the spin-split bands of ferromagnetic metals. We show below that it is this third term that makes coupling between spins and charges.

To solve for the spin-dependent potential and induced charge density, it is necessary to model the dielectric response. In the case of a weak external electric field, one may consider a linear relation between the induced charge and the spin-dependent potential,

$$\delta n^\sigma(x) = \int R^\sigma(x,x')V^\sigma(x')\,dx', \tag{5}$$

where $R^\sigma(x,x')$ is the charge-density response kernel and $V^\sigma(x) = V_c(x) + (J/e)[\delta n^\sigma(x) - \delta n^{-\sigma}(x)]$ is the induced spin-dependence potential. By combining Eqs. (3) through (5), we find

$$\delta n^\uparrow(x) - \delta n^\downarrow(x) = \int D(x,x')V_c(x')dx' - \frac{J}{e}\int S(x,x')[\delta n^\uparrow(x') - \delta n^\downarrow(x')]\,dx' \tag{6}$$

and

$$\frac{d^2V_c(x)}{d^2x} = -\frac{e}{\epsilon_0}\int S(x,x')V_c(x')\,dx' + \frac{J}{\epsilon_0}\int D(x,x')[\delta n^\uparrow(x') - \delta n^\downarrow(x')]\,dx', \tag{7}$$

where we have defined the difference and the sum of the response kernels for two spin channels, i.e., $D(x,x') = R^\uparrow(x,x') - R^\downarrow(x,x')$ and $S(x,x') = R^\uparrow(x,x') + R^\downarrow(x,x')$. Thus, the problem of the surface screening is reduced to solving the above complex integrodifferential equations. Equation (6) describes the induced magnetization and Eq. (7) the charge buildup. To solve these coupled equations, appropriate boundary conditions and explicit forms of the response kernels are needed.

First, consider boundary conditions in two interesting experiments. One is for spin-polarized field emission experiments where the electric field is directly applied to the ferromagnet surface. Then, the spin polarization of the emitted electrons from the surface is measured. In this case for an applied field E_0 the boundary condition takes the form, i.e.,

$$\frac{dV_c(0)}{dx} = -E_0 \tag{8}$$

at the surface $x = 0$ and $V_c(x) = 0$ deep inside the metal.

In a magnetic tunnel junction, one applies a voltage V_a across the junction. Assuming the electric field is uniform inside the insulator barrier, the boundary condition becomes

$$\epsilon_0\frac{dV_c(0)}{dx} = \epsilon_0\frac{dV_c(t)}{dx} = \epsilon_i\frac{V_c(t) - V_c(0)}{d}, \tag{9}$$

and $V_c(\infty) - V_c(-\infty) = V_a$, where the two interfaces are at $x = 0$ and at $x = t$; ϵ_i is the effective dielectric constant of the insulator barrier, and we have assumed that the magnetic electrodes at both sides of the insulator barrier are identical. Clearly, this case is not as simple as that of the field emission case, since it involves both the potential and the derivative of the potential at interfaces.

Next we model the kernel $R^\sigma(x,x')$ using the random phase approximation (RPA). Within a free electron model, the response function for each spin band is

$$R^\sigma(x,x') = -\left(\frac{mk_F^\sigma e^2}{\hbar^2\pi^2}\right)\int dy\left[\frac{1}{2} + \frac{1-y^2}{4y}\ln\left|\frac{1+y}{1-y}\right|\right]e^{2ik_F^\sigma(x-x')y}, \tag{10}$$

where k_F^σ is the Fermi wave vector of spin σ. With this explicit expression of the kernel and the boundary conditions, Eqs. (8) or (9), one can determine the charge buildup $\delta n^\sigma(x)$. While the structure of the above equations bears very much in common with the spin-polarized coupling across *nonmagnetic* spacers, there are several interesting distinctions:

(1) While the usual spin density waves are generated by *spin-dependent* perturbations at the interface for a nonmagnetic metal, they can be generated by *spin-independent* perturbations (external electric fields) for a *ferromagnet*. (2) Similar to Friedel and RKKY oscillations, charge and magnetization oscillate with the period determined by Fermi wave vectors $k_F^{\uparrow}$ and $k_F^{\downarrow}$. However, the induced charge and magnetization contain multiple periods such as $2\pi/(k^{\uparrow} + k^{\downarrow})$ and $2\pi/(k^{\uparrow} - k^{\downarrow})$ because the spin-up and spin-down electrons are coupled in Eqs. (8) and (9).

While the RPA is a valid approximation to study the asymptotic behavior of the induced charge density, the local response is useful to understand the screening at the first monolayer of the surface. In a magnetic tunnel junction, the electronic structure at the very first layers determines the tunneling characteristics. Therefore, this case has direct relevance to the recently discovered voltage dependence of the spin-polarized tunneling in MTJ [6]. In the linearized Thomas-Fermi model, the kernel is

$$R^{\sigma}(x,x') = -e\rho^{\sigma}(\epsilon_F)\delta(x - x'), \tag{11}$$

where $\rho^{\sigma}(\epsilon_F)$ is the density of states at the Fermi level for spin σ. While the Thomas-Fermi is a rather crude approximation and it gives poor quantitative values, our intention is to illustrate the importance of the spin-dependent screening on the spin-polarized effects. This approximation gives an exact solution of our problem and qualitative estimations can be readily carried out. With this local relation, Eqs. (6) and (7) reduce to simple differential equations,

$$\delta n^{\uparrow}(x) - \delta n^{\downarrow}(x) = -\frac{\rho^{\uparrow} - \rho^{\downarrow}}{1 + J(\rho^{\uparrow} + \rho^{\downarrow})}\, eV_c(x) \tag{12}$$

and

$$\frac{d^2V_c(x)}{dx^2} = \frac{1}{\lambda^2}\, V_c(x), \tag{13}$$

where we define the screening length as

$$\lambda = \left\{\frac{e^2}{\epsilon_0}\,\frac{\rho^{\uparrow} + \rho^{\downarrow} + 4J\rho^{\uparrow}\rho^{\downarrow}}{1 + J(\rho^{\uparrow} + \rho^{\downarrow})}\right\}^{-1/2}. \tag{14}$$

In a nonmagnetic metal where $\rho^{\uparrow} = \rho^{\downarrow}$ and $J = 0$, the above equation reduces to the conventional Thomas-Fermi screening length, $\lambda_N = (e^2\rho/\epsilon_0)^{-1/2}$, where ρ is the density of states. In the presence of exchange interactions and spin polarization ($\rho_{\uparrow} \neq \rho_{\downarrow}$), it is easily seen from Eq. (14) that the Thomas-Fermi screening length is enhanced, i.e., $\lambda > \lambda_N$. A quite long Thomas-Fermi screening length can be realized in systems with large asymmetric spin-dependent densities of states, e.g., if the exchange constant J is large and if $\rho^{\uparrow} \gg \rho^{\downarrow}$. To qualitatively estimate the size of the effect, we use *bulk* Ni, Co, and Fe [8] even though the electronic structures of the surfaces are expected to be different from the bulk. We take the exchange parameter J to be the same as used by others [7]. The Thomas-Fermi screening lengths in Ni, Co, and Fe calculated from Eq. (14) are given in column five.

If one applies this local response screening to a magnetic tunnel junction, Eq. (13) has a simple solution $V_c(x) = V_c(0)\exp(x/\lambda)$ for the left electrode and $V_c(x) = V_a - [V_a - V_c(t)]\exp[-(x - t)/\lambda]$ for the right electrode, where V_a is the applied voltage and t is the thickness of the insulator layer. By using the boundary condition given by Eq. (9), one can easily determine $V_c(0)$,

$$V_c(0) = \frac{\epsilon_i\lambda V_a}{\epsilon_0 t + 2\epsilon_i\lambda}, \tag{15}$$

where we have assumed that the left and right electrodes are identical. The total magnetization accumulation at the left electrode per interface atom is found by integrating Eq. (12) to be

$$\begin{aligned}\delta M_{\mathrm{acc}} &= \int_{-\infty}^{0}(\delta n^{\uparrow} - \delta n^{\downarrow})\mu_B\,dx\\ &= \frac{\epsilon_0\epsilon_i(\rho^{\downarrow} - \rho^{\uparrow})\mu_B V_a}{e^2(\rho^{\uparrow} + \rho^{\downarrow} + 4J\rho^{\uparrow}\rho^{\downarrow})(\epsilon_0 t + \epsilon_i\lambda)},\end{aligned} \tag{16}$$

and the difference of the potentials for spin up and down is

$$V^{\uparrow}(x) - V^{\downarrow}(x) = \frac{2J(\rho^{\downarrow} - \rho^{\uparrow})V_c(0)\exp(x/\lambda)}{1 + J(\rho^{\downarrow} + \rho^{\uparrow})}. \tag{17}$$

If one interprets that $V^{\sigma}(0)$ is the voltage absorbed in the electrode, the above equation shows the spin dependence of the voltage absorption. Therefore, one anticipates that the effective barrier seen by conduction electrons is different for spin up and down. This will affect the spin-dependent tunnel rates, as we will show below. In the last two columns of Table I, we list the average voltage for spin up and down absorbed in the electrodes, and the magnetization accumulation at the interface for Ni, Co, and Fe electrodes.

The induced screening charges and magnetization have several immediate consequences. First, the capacitance of a junction departs from its geometrical capacitance, $C_0 = \epsilon_i A/t$, since part of the applied voltage is absorbed by the electrodes. This phenomenon had been first discussed in nonmagnetic metals [9]. The reduction of the capacitance from its classical value can be quite significant for thin insulator barriers. For example, the capacitance of the junction is reduced by factor of 2 for a device which has an insulator layer thickness of 24 Å and Co electrodes; see column six of Table I. Second, the magnetization accumulation will affect the spin polarization of the tunnel currents. To see this, we note that the tunnel current is primarily governed by interface electronic structures which are altered by the presence of spin-dependent band

TABLE I. Parameters extracted from bulk band structures of Ni, Co, and Fe: J values were taken from Ref. [8] and $\rho^{\uparrow,\downarrow}$ from Ref. [7]. λ's were calculated from Eq. (14), $V_c(0)/V_a$ from Eq. (15). t is the barrier thickness in units of Å, the dielectric constant was assumed to be 8, and V_a is in units of volts, δM_{acc} is the induced magnetic moment per interface atom.

Electrode	E_{ex}(eV)	$\rho^{\uparrow}(\mathrm{eV})^{-1}$	$\rho^{\downarrow}(\mathrm{eV})^{-1}$	λ(Å)	$2V_c(0)/V_a$	$\delta M_{\mathrm{acc}}/\mu_B$
Ni(fcc)	0.65	0.18	1.56	0.9	$14.4/(t + 14.4)$	$0.12V_a/(t + 14.4)$
Co(hcp)	1.25	0.18	0.70	1.5	$24.0/(t + 24.0)$	$0.088V_a/(t + 24.0)$
Fe(bcc)	2.40	0.87	0.24	1.3	$20.8/(t + 20.8)$	$-0.044V_a/(t + 20.8)$

bending at the interfaces, i.e., the absorbed voltage is different for spin up and down electrons; see Eq. (17). Thus, one anticipates that this effect contributes to the voltage dependence of the magnetoresistance in MTJ. Quantitative calculation will depend on models used for electron tunneling [10].

Finally, we wish to comment on the effect of our spin-dependent field penetration on spin-polarized field emission experiments. In such experiments, an applied voltage with typical magnitude of the order of a few volts is directly applied to a magnetic surface. To assure adequate electron emission, the separation between the surface and the tip must be small, usually only a few angstroms. Thus, the electric field is quite strong at the emitting surface and one anticipates that measured spin polarization of the emitting current depends sensitively on the separation between the surface and the tip. Indeed, different experimental groups have observed quite different spin-polarization data for the same Ni samples [11]. This can be interpreted as due to a subtle difference in electric fields used by different groups. For example, one may estimate the voltage dependence of the emitting spin current I^{σ} by a simple direct tunnel formalism as $I^{\sigma} = i_0^{\sigma} \exp[-sK\sqrt{(\phi - eV^{\sigma})}]$ where i_0^{σ} is related to the spin resolved density of states, s is the separation between emitting surface and the tip, ϕ is the effective average barrier height without taking into account the field penetration, and K is related to the effective mass of tunnel electrons. By taking reasonable parameters, e.g., $K = (1\ \text{Å}^{-1})(V)^{-1/2}$, $\phi = 3$ eV, and $V_a = 2$ eV, the spin polarization of the emitting current changes significantly by decreasing the distance s from 7 to 5 Å (in this example, it will be 50%). This dramatic change has been reported experimentally by Alvarado [12].

In summary, we have studied electron screening in ferromagnetic surfaces in applied electric fields. The screening potential has an important spin-dependent contribution. The interplay of the screening due to Coulomb and exchange interactions was analyzed. A complicated integrodifferential equation which governs the surface charge and magnetization buildup was derived. Within a local response approximation, the equation was solved for a magnetic tunnel junction. In addition, nonequilibrium charge and magnetization accumulations were estimated for Ni, Co, and Fe.

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