Impact of interfacial roughness on spin filter tunneling

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The impact of interface roughness on spin filter tunneling is considered at low biases as functions of temperature and barrier parameters. Roughness reduces the maximum achievable spin polarization, which results from tunneling "hot spots" (thin regions of the barrier) having intrinsically reduced spin filtering efficiency. Surveying a range of experimentally reasonable roughness and mean barrier thickness values allows us to conclude that roughness values greater than 10% of the mean barrier thickness have an adverse impact on the spin polarization. Atomic-scale roughness may thus be critical for achieving 100% spin polarization in spin filter tunnel junctions at low biases. © *2010 American Institute of Physics*. [doi:10.1063/1.3291065]

Spin filter tunneling (SFT) represents one way of achieving highly spin polarized currents.[1] Perhaps the most intriguing implication of SFT is the ability to generate spin polarized currents using electrodes that are nonmagnetic, and potentially even nonmetallic. In SFT junctions, the tunneling current is spin polarized because spin up and spin down electrons have different tunneling probabilities, which is a consequence of exchange splitting of the tunnel barrier material leading to spin-dependent barrier heights. The temperature dependence of this polarization process follows that of the exchange splitting of the spin filter material.[2] In addition to the four barrier height parameters, the barrier thickness plays an important role in SFT junctions.[3] By surveying the entire SFT barrier parameter space at low biases, it was recently concluded that the barrier thickness plays a critical role in spin filtering as follows: increasing the barrier thickness increases the maximum achievable spin polarization level, and allows a given spin polarization to be reached at higher temperatures (assuming single step tunneling).[3] Of course, the thickness cannot be increased without potentially major costs, including impractically large tunneling resistances potentially accompanied by the onset of multistep tunneling, and appreciable interfacial roughness. The latter cannot be avoided during the growth of multilayered heterostructures, even in epitaxial systems.[4] It is well known at this point that roughness is a critical parameter in many varieties of tunneling junctions,[5–8] but this has yet to be addressed in SFT. In this letter, we investigate the impact of experimentally reasonable roughness values on SFT, using established tunneling formalisms with distributions of barrier thicknesses to simulate roughness.

There are two fundamental parallel conduction channels in spin filter junctions, one for each spin. The net current density is the average of the spin up and spin down current densities $j_{\mathrm{net}}=(j_\uparrow+j_\downarrow)/2$. Spin up and spin down electrons see different barrier heights below the ordering temperature of the magnetic insulator, $\phi_\uparrow$ and $\phi_\downarrow$, respectively. The spin channel with the lower barrier height has a larger transmission coefficient, which implies that the current entering the collector electrode is spin polarized. This polarization is typically expressed as $P=(j_\uparrow-j_\downarrow)/(j_\uparrow+j_\downarrow)$, where the spin-dependent current densities are calculated using spin and temperature dependent barrier heights. We calculate the tunneling current density for each spin channel using an expansion of the model of Brinkman, Dynes, and Rowell[9] as

$$j(\varphi) = G_{\mathrm{o}}\left(V + \frac{s\sqrt{2m/q}\Delta\varphi}{24\hbar\bar{\varphi}^{3/2}}V^2 + \frac{s^2 mq}{12\hbar^2\bar{\varphi}}V^3\right), \tag{1}$$

where the leading term is the tunneling conductance at zero bias

$$G_{\mathrm{o}}(\varphi) = \left(\frac{q}{h}\right)^2\sqrt{\frac{2mq\bar{\varphi}(0\ \mathrm{V})}{s^2}}\exp\left[\frac{-2s}{\hbar}\sqrt{2mq\bar{\varphi}(0\ \mathrm{V})}\right].$$

Here, φ relates to either spin channel ($\varphi=\phi_\uparrow$ or $\phi_\downarrow$). Thus, for either spin channel $\bar{\varphi}$ is the position, bias, and temperature dependent average barrier height; $\Delta\varphi$ is the interfacial barrier height difference at zero bias; s is the barrier thickness; q is the elementary charge; and m is the electron mass; all in SI units. This expansion is only valid for biases small relative to the barrier height; it was previously determined that "small" biases are those less than roughly one third of the barrier height,[7] above which higher order terms take over as the Fowler–Nordheim tunneling regime is approached. Assuming the exchange splitting is proportional to the magnetization allows us to define the spin dependent barrier heights above and below the magnetic ordering temperature, T_{c}

$$T \le T_{\mathrm{c}}: \begin{cases} \phi_\uparrow = \phi_{\mathrm{o}} - \Delta E_{\mathrm{ex}}\sqrt{1-T/T_{\mathrm{c}}} \\ \phi_\downarrow = \phi_{\mathrm{o}} + \Delta E_{\mathrm{ex}}\sqrt{1-T/T_{\mathrm{c}}} \end{cases},$$

$$T > T_{\mathrm{c}}: \varphi = \phi_{\mathrm{o}}. \tag{2}$$

This temperature dependence captures the behavior near the critical temperature well for localized moments, and sufficiently well at low temperatures to understand the impact roughness has on SFT. The culmination of these features is that the zero-bias resistance-area product (i.e., $1/G_{\mathrm{o}}$) drops dramatically as the temperature falls below T_{c}, which is a direct consequence of the spin-up barrier height decreasing with decreasing temperature, as per Eq. (2). Further, the polarization increases with decreasing temperature, which results from the exchange splitting continuously approaching its zero temperature value.

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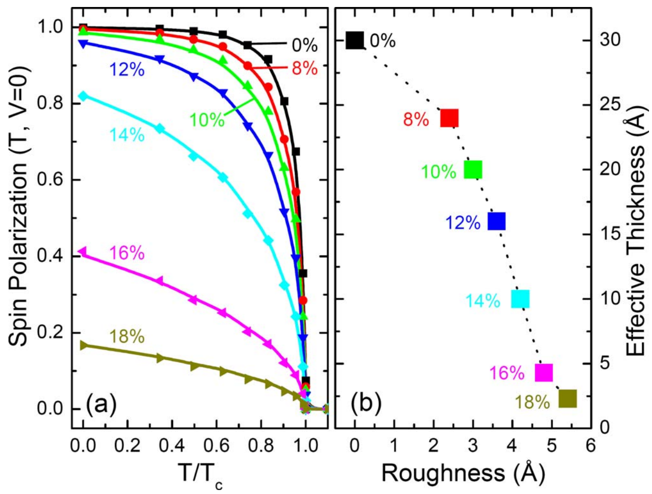

FIG. 1. (Color online) (a) Temperature dependence of spin polarization for a junction with $\phi_o=1$ eV, $2\Delta E_{ex}=0.5$ eV, and $\bar{s}=30$ Å in the presence the indicated roughness values (in percent of $\bar{s}$). Data symbols are calculated with roughness; lines are fits with ideal (i.e., no roughness) temperature dependence. The best fit effective thicknesses are shown in (b) (dotted line is a guide to the eye).

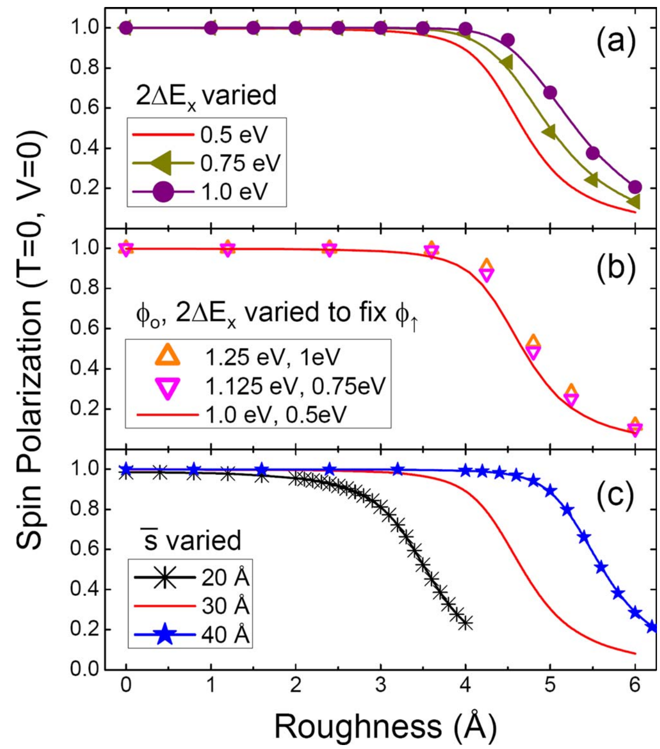

FIG. 2. (Color online) Roughness dependence of spin polarization for spin filter junctions with the following nominal parameters: $\phi_o=1$ eV, $2\Delta E_{ex}=0.5$ eV, and $\bar{s}=30$ Å. In each panel, the red solid line is the performance of the nominal junction. The sensitivity of the polarization to roughness is (a) slightly decreased with increased exchange splitting, (b) nearly independent of barrier height parameters if the spin-up barrier height is held constant, and (c) strongly dependent on mean thickness.

To simulate the effect of roughness on SFT, we calculated the current density via Eq. (1) for a distribution of barrier thicknesses s_n by weighting each individual current density $j(s_n,\varphi)$ with a thickness-dependent coefficient and summing these as parallel conduction channels. The net conductance G_{net} was obtained from the net current density $j_{net}=\Sigma_n\alpha(s_n)j(s_n,\varphi,V)$, with the n^{th} channel weighted by a coefficient $\alpha(s_n)$ that is obtained from the Gaussian distribution of thicknesses centered at mean thickness $\bar{s}$ with the standard deviation σ defining the roughness. The distribution $s_n=\bar{s}\pm\sigma$ represents variations of the barrier thickness over the entire junction area and at both interfaces. One can interpret the weighting coefficients as the relative area of each conduction channel.[10] A thickness step size of 0.5 Å was used because the results were independent of Δs less than this value. While this formalism is general for asymmetric barriers, we assume symmetric barrier heights at zero bias for computational ease. Additionally, we do not consider barrier height distributions, though such distributions are known to exist in tunnel junctions.[11] The main impact of a distribution of barrier heights is to lower the junction's effective barrier height,[12] and is intrinsically less significant than thickness distributions because the barrier height is under the radical in the tunneling exponent ($e^{-s\sqrt{\phi}}$).

Figure 1(a) shows the temperature dependence of the spin polarization of a junction with $\phi_o=1$ eV, $2\Delta E_{ex}=0.5$ eV, and $\bar{s}=30$ Å in the presence of various amounts of roughness. We use these barrier parameters for the nominal junction throughout this work, as they are representative of experimentally demonstrated spin filter materials such as EuO.[1] Relative to an ideal junction ($\sigma=0$), roughness suppresses the temperature dependence. In fact, each data set generated with nonzero roughness is fit well by the temperature dependence of an ideal junction whose thickness is thinner than $\bar{s}$. Citing the exponential dependence on the barrier thickness, thinner regions of the barrier dominate the tunneling conductance and lead to an effective thickness less than the mean thickness. As shown in Fig. 1(b), this effective thickness is a strong function of roughness. As noted in previous roughness studies,[13] the specific values reported here are functions of each of the barrier parameters used, though the basic functionality will be retained with different barrier parameters.

Relative to the nominal junction, Fig. 2 summarizes the impact of roughness on the low temperature, low bias spin polarization of junctions with a variety of barrier parameters. The general behavior of the spin polarization is to fall rapidly once roughness becomes important as follows: P falls by 90% or more within a roughness range of about 2 Å for any combination of parameters studied. Thus, it appears that the barrier parameters strongly influence the roughness levels leading to the decay of P, but weakly influence the functionality of the decay. The roughness leading to a reduction in polarization by one-half, σ_c, is useful for characterizing the position of the transition. As shown in Fig. 2(a), there is only a slight dependence on the exchange splitting, with a doubling of 2Δ increasing σ_c by less than 1 Å. Figure 2(b) shows that σ_c is nearly unchanged if the lower spin barrier height, $\phi_\uparrow$ in this case, is held constant (for a given thickness). Together, these results suggest that $\phi_\uparrow$ is the only barrier height parameter that strongly influences the sensitivity of the polarization on roughness. This is quite reasonable because the lower height channel dominates the tunneling conductance.

The parameter with greatest influence on the spin polarization's sensitivity to absolute roughness is the mean barrier thickness. Figure 2(c) shows that the spin polarization decreases systematically with increasing roughness for mean thicknesses of 20, 30, and 40 Å, which are three relevant

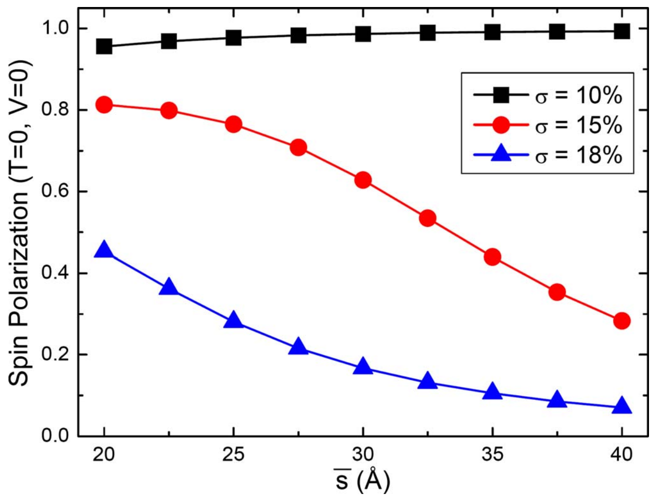

FIG. 3. (Color online) (a) Mean thickness dependence of spin polarization for junctions with ϕ_o=1 eV, $2\Delta E_{ex}$=0.5 eV, for the indicated roughness parameters.

thicknesses for tunneling junctions. For each $\bar{s}$, the spin polarization decays rapidly as above, within a window of about 2 Å. The σ_c values increase with $\bar{s}$, extending from around 3.5 Å for $\bar{s}$=20 to 5.5 Å for $\bar{s}$=40 Å. It is apparent that the tunneling spin polarization is significantly decreased for experimentally reasonable barrier thicknesses with modest roughness values of 3–6 Å. The existence of these levels of roughness is very plausible if not unavoidable,[6,14,15] and is likely a leading cause of the difficulty in demonstrating 100% spin polarization in spin filter junctions. Such deleterious effects on polarization could potentially be overcome by accessing the Fowler–Nordheim regime of the lower spin channel barrier with high applied biases.[16,17]

It is further illustrative to analyze the tunneling spin polarization as a function of mean thickness for constant roughness percentages, as in Fig. 3. The roughness parameters range from 10%–18% of the mean thicknesses, representing experimentally achievable values. For values of roughness near and below 10% of the mean thickness, the maximum achievable spin polarization increases with thickness. This behavior is indicative of an ideal junction,[3] and implies little impact of roughness on the spin filtering process. As roughness increases, however, the effective barrier thickness is reduced [Fig. 1(b)], which in turn causes a decline in spin polarization. It is worth noting that for most materials of current interest, the minimum roughness that leads to a reduced spin polarization is around one unit cell, which should underscore the importance of low roughness barriers in SFT.

In conclusion, we have considered the impact of roughness on the spin filtering process in SFT using parameters characteristic of current materials of interest, such as EuO. Roughness reduces the effective thickness of the barrier, which ultimately leads to a reduced spin filtering efficiency. Roughness values exceeding 10% of the mean thickness tend to reduce the maximum achievable spin polarization, with this reduction amplified for thicker barriers. Because roughness is experimentally difficult to avoid, this quality may be a leading cause of the difficulty in obtaining 100% spin polarization at low biases in SFT.

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