Inherent temperature effects in magnetic tunnel junctions

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Theoretical studies of the temperature dependence of the tunneling magnetoresistance ratio (TMR) are presented. A successful elastic tunneling model has been extended to handle temperature dependence. It treats Fermi smearing and applies Stoner-like behavior to the exchange split band structure in the electrodes to calculate TMR(T). As expected, the effects of Fermi smearing are small, but small changes in the magnetic band structure produce large changes in TMR. For a Co/I/Co junction produced by LeClair *et al.* [Phys. Rev. Lett. **84**, 2933 (2000)], calculations using bulk magnetization predicted 33% of the experimental loss of TMR from 0 to 300 K with only a 1.5% change in magnetization. A mere 3.2% change in magnetization produced 100% of the observed drop in TMR. These results imply larger than imagined intrinsic temperature dependence for TMR. [DOI: 10.1063/1.1357126]

Originally, extrinsic mechanisms were favored to explain the temperature dependence of TMR [Δ TMR(T)] because Fermi smearing and the temperature dependence of magnetization [$\Delta M(T)$] for 3*d* ferromagnets are mild below 300 K.[1,2] In 1998, Zhang and White[1] proposed that the temperature dependence of TMR could be explained by spin-independent two-step tunneling via defect states in the barrier. Moodera *et al.*[3] suggested that ΔTMR(T) can be explained by the temperature dependence of the surface magnetization of the leads which is more dramatic than bulk magnetization. Shang *et al.*[4] modified Julliere's model[5] with a spin-independent conductance channel and temperature dependent polarization, $P(T)$. They concluded that direct elastic tunneling with a Bloch law dependent polarization was the dominant factor in TMR(T).

Shang started with Julliere's general formula.[5] However, Julliere's model is rarely exact[6] and lacks the ability to predict temperature, bias, or barrier dependence because it ignores the details of the barrier by simply treating it with spin-independent matrix elements. On the other hand, our model produces spin-dependent matrix elements and extends a successful free electron model[7] similar to one proposed by Slonczewski,[8] treating both barrier thickness as well as barrier height. Spin dependence arises not from a spin-dependent barrier *per se*, but rather from matching spin polarized states in the leads to spin-independent states in the barrier.

Free electron-like bands near E_f in ferromagnets are thought to be responsible for tunneling in magnetic tunnel junctions (MTJs).[9,10] These can be modeled by exchange split parabolic bands with density of states (DOS) proportional to

$$k_i=\sqrt{2m_i^*(E-V_i)}, \tag{1}$$

where m_i^* is the effective mass and V_i is the bottom of each band. Recent evidence shows that these bands are Stoner-like.[11,12] Therefore, the exchange splitting depends on temperature and collapses near T_c. Shimizu *et al.*[13] showed that exchange splitting is nearly proportional to $M(T)$. The proportionality constant β is mildly dependent on T, but varies so slowly that it can be considered a constant below room temperature. For instance, the change in β for iron is only about 2.5% between 0 and 300 K. Therefore we expect this assumption to slightly overestimate the exchange splitting because $d\beta/dT$ is negative. Assuming exchange splitting proportional to $M(T)$ for a typical system yields

$$\Delta E_{\rm ex}=\beta M(T)=[V_\downarrow(T)-V_\uparrow(T)]. \tag{2}$$

Using Eq. (1) and the usual definition of P,[6]

$$P(T)=\frac{\sqrt{2m_\uparrow^*[E-V_\uparrow(T)]}-\sqrt{2m_\downarrow^*[E-V_\downarrow(T)]}}{\sqrt{2m_\uparrow^*[E-V_\uparrow(T)]}+\sqrt{2m_\downarrow^*[E-V_\downarrow(T)]}}, \tag{3}$$

where $V_\uparrow(T)=-\Delta E_{\rm ex}/2$ and $V_\downarrow(T)=+\Delta E_{\rm ex}/2$. The zero of potential is the bottom of the resulting paramagnetic band at T_c.

For specific MTJs, we used published bulk magnetization curves.[14] Intrinsic to these curves is the effect of magnons and other excitations on the temperature dependence of the magnetization in the leads. We used a set of parabolic bands with the same exchange splitting and effective mass as tunneling bands calculated from first principles. Both exchange splitting and the difference in effective masses are allowed to relax with increasing temperature.[11,15,16] We assume a step barrier with parameters deduced from the experiment. An applied voltage drops smoothly in the barrier forming a sloping barrier. The DOS are modified by Fermi–Dirac statistics and used to calculate parallel and antiparallel conductances to determine TMR(T) using the barrier T matrix.[17,18] The results of calculations for a typical Co/I/Co system are displayed in Figs. 1 and 2.

To facilitate a qualitative comparison, we have plotted TMR/TMR$_{\rm max}$, $P/P_{\rm max}$ and $M/M_{\rm max}$. In Fig. 1, P is nearly proportional to the magnetization. This near proportionality

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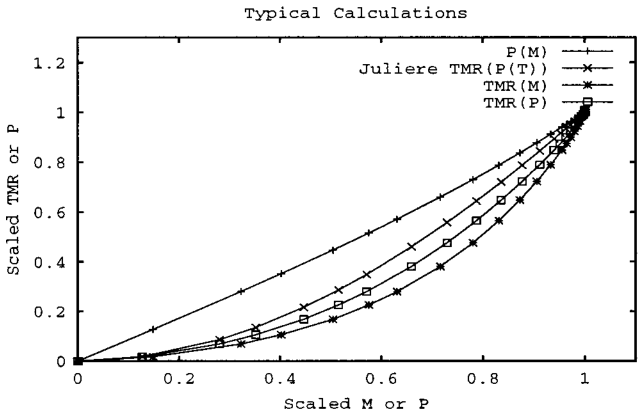

FIG. 1. Calculations for a typical Co/I/Co MTJ using bulk magnetization.

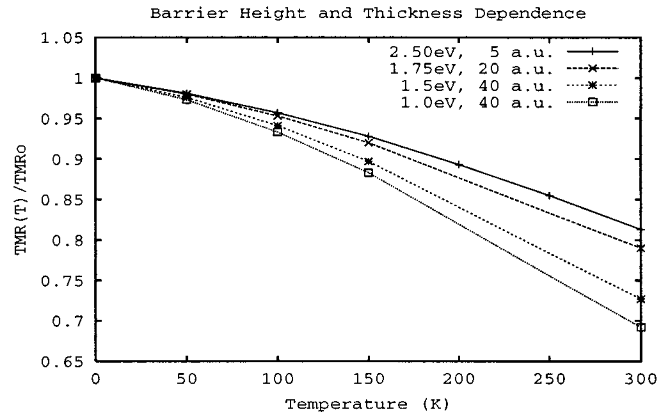

FIG. 3. TMR(T) for various barriers. High thin barriers give milder ΔTMR(T).

is associated with the coincidentally small curvature of the bands near the Fermi level. However, dP/dM is slightly larger at greater M (lower temperature), and $d(\mathrm{TMR})/dM$ shows a similar but exaggerated behavior. We see a large (small) sensitivity to small changes in M at low (high) temperature.

Figure 2 shows the comparison between our model and Julliere's formula using a temperature dependent polarization. Our model produces greater ΔTMR(T). For instance, Julliere's modified formula predicts a drop in TMR of 11.2% when the magnetization changes by 5.0% while the tunneling calculation predicts a drop of 16.4%. At higher temperatures $d(\mathrm{TMR})/dT$ for the model may actually be less than dP/dT.

The difference between the two models is the way in which the effect of the barrier is handled. The different predictions of the two implies that the results are sensitive to the barrier description. Figure 3 shows the effect of varying barrier geometry on TMR(T) where high-thin barriers give milder ΔTMR(T).

We can explain the barrier sensitivity of TMR in terms of spin-dependent matrix elements which come from matching spin-dependent states with spin-independent barrier states at two interfaces a finite distance apart. The barrier states depend on the barrier height. Our model only distinguishes between spins insomuch as the tunneling states originate from different bands, so the magnitude of the spin-dependent barrier effect should be related to the degree of dissimilarity between the bands. Therefore we expect maximum barrier effect for maximum splitting (low temperature) and minimum effect as the bands converge at high temperature. This would account for the qualitative differences between $M(T)$ and TMR(T) where we see that $d(\mathrm{TMR})/dT$ is greater than $dM(T)/dT$ at low temperature, can be similar to $dM(T)/dT$ at intermediate temperatures, and is less than $dM(T)/dT$ at high temperatures. In fact, a calculation using iron which has greater $\Delta M(T)$ and lower T_c produces a bell-shaped curve. Figure 4 shows that the temperature dependent band structure contributes more strongly to the temperature dependence than does Fermi smearing. Figure 5 compares the model with data from a Co/Al_2O_3/Co junction by LeClair *et al.*[19]

LeClair's MTJs were prepared by ultrahigh vacuum dc/rf magnetron sputtering ($<5\times10^{-10}$ mbar) through metal contact masks on Si(100). *In situ* cleaning in O_2 plasma was used to remove contamination and produce insulation from substrates. Barriers were formed by plasma oxidation of 2 nm Al in 10^{-1} mbar O_2. A uniform exchange biasing direction was promoted by annealing in a magnetic field. *In situ* x-ray photoelectron spectroscopy and *ex situ* optical techniques confirmed no Co oxidation and minimal metallic Al. *In situ* scanning tunneling microscopy on control samples indicated flat films, small grains, and a mean roughness of

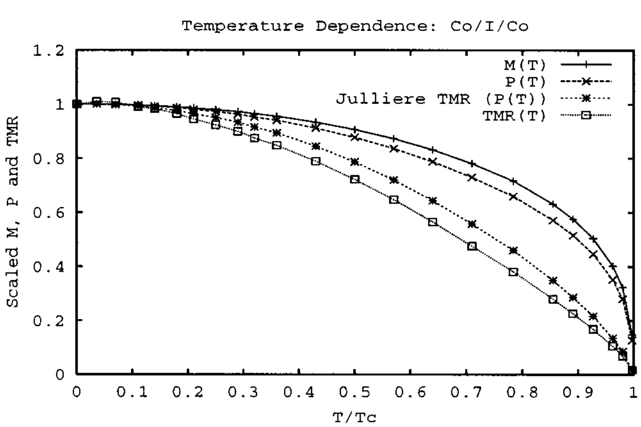

FIG. 2. Theoretical TMR(T),$P(T)$ using bulk $M(T)$ for cobalt. Julliere's TMR calculated using $P(T)$.

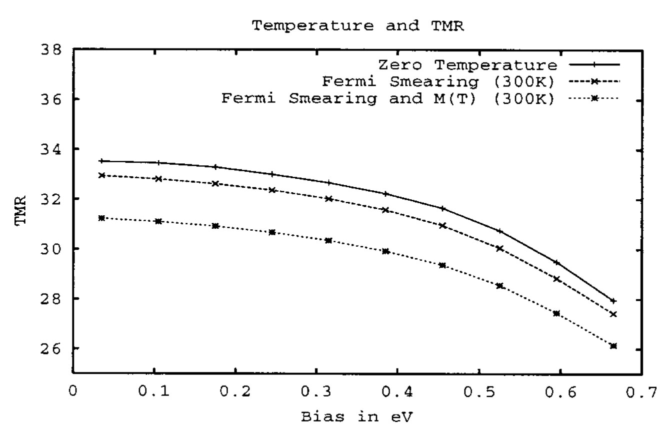

FIG. 4. The effect of Fermi statistics.

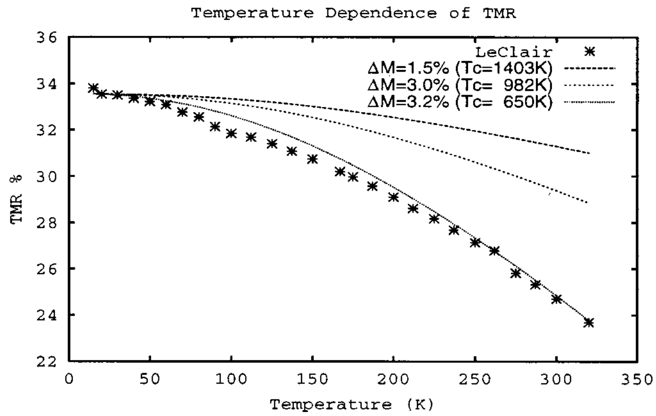

FIG. 5. Calculated TMR(T) compared to experiment. The top curve uses the bulk magnetization curve for cobalt. $T_{c\mathrm{Co}}=1402$ K. The middle curve assumes a 30% reduction in T_c to 982 K. T_c has been adjusted to fit the data for the bottom curve. The total change in M from 0 to 300 K was 3.2%.

<0.3 nm. Resistances (*dV/dI*) were measured using standard ac lock-in techniques, while TMR ($\Delta R/R_p$) was measured using dc and ac lock-in techniques.

Conservative calculations using bulk magnetization (top curve) account for 33% of the observed drop for LeClair's data. The data was fit by making T_c an adjustable parameter and renormalizing the magnetization. The second curve assumes a 30% reduction in T_c as suggested by Bander and Mills.[20] To put things in perspective, renormalizing $M(T)$ so that the change in magnetization is 3.2% from 0 to 300 K (bottom curve) produces 100% of the observed drop. Similar results were obtained for a NiFe/Al_2O_3/NiFe junction fabricated by Matsuda *et al.*[21] where 36% of the drop in TMR is produced by the bulk magnetization curve, and the change of magnetization at 300 K required to fit the data was 7.8%. The T_c yielded by renormalizing should not be construed to have any relationship to the actual T_c at the interface since renormalizing bulk magnetization to a lower T_c is simply a strategy to introduce slightly greater dM/dt and simulate a less bulk-like magnetization curve. The magnetization at an interface is expected to be intermediate to bulk and surface magnetization because of the presence of the barrier. The actual magnetization curve at the interface is expected to more simply produce this result.

In conclusion, a large intrinsic ΔTMR(T) is the result of the tunneling process. The temperature dependence originates in the temperature dependence of the magnetic band structure and is very sensitive to the barrier because of the T matrix which results from the matching of states at the interfaces. The temperature dependence should be greatest at low temperature where exchange splitting is maximum, but high T_c produces milder ΔTMR(T) because $\Delta M(T)$ is milder. More surface-like magnetization produces the best fit to the experimental signature.

Finally, the assumption of bulk-like magnetization and exchange splitting proportional to $M(T)$ likely underestimates the importance of the intrinsic ΔTMR(T). Therefore due to its large sensitivity to small changes in the magnetic structure, large enhancements of TMR can be leveraged by small enhancements of magnetization.

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