

Impurity-Induced Tuning of Quantum-Well States in Spin-Dependent Resonant Tunneling

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We report exact model calculations of the spin-dependent tunneling in double magnetic tunnel junctions in the presence of impurities in the well. We show that the impurity can tune selectively the spin channels giving rise to a wide variety of interesting and novel transport phenomena. The tunneling magnetoresistance, the spin polarization, and the local current can be dramatically enhanced or suppressed by impurities. The underlying mechanism is the impurity-induced shift of the quantum well states (QWSs), which depends on the impurity potential, impurity position, and the symmetry of the QWS.

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Tunneling of spin-polarized electrons through magnetic tunnel junctions (MTJ) has attracted [1] wide and sustained interest in the past few years, both experimentally [2–6] and theoretically [3,7–9]. This is due to the potential applications of MTJ in spin-electronic devices, such as magnetic sensors and magnetic random-access memories. The key point for these applications is the tunnel magnetoresistance (TMR), i.e., the dependence of the tunneling current on the relative orientation of the magnetization of the ferromagnetic layers, which can be changed by an applied magnetic field [6].

Double magnetic tunnel junctions (DMTJ) consist of a central metallic layer between two insulating barriers and two ferromagnetic electrodes. The insulating layers are thin enough for electrons to tunnel through the barriers if a bias voltage is applied between the electrodes. The TMR behavior in DMTJ is determined by quantum well states (QWS) formed in the middle layer when a resonance condition is fulfilled [5]. The TMR can be dramatically enhanced when spin-polarized electrons *resonantly* tunnel through the middle layer [7]. Theoretical formulations of the TMR in DMTJ are usually based on models which assume perfect systems [7,9–14]. The TMR exhibits an amplitude-varying oscillatory behavior as a function of the thickness of the middle layer with a period of π/k_F^{σ} , where k_F^{σ} is the spin-dependent Fermi wave vector in the middle layer [10]. Chshiev *et al.* [9] introduced an effective electric field within each barrier in order to satisfy the continuity equation for the current [15].

However, actual MTJ contain large amounts of disorder in the electrodes, in the barriers, in the quantum well, and at the electrode/barrier or electrode/quantum well interfaces [3,16]. Experiments in single MTJ have suggested that disorder can affect the TMR in a critical way, giving rise to impurity-assisted tunneling [3,16]. While the effect of impurities within a single barrier has been recently studied theoretically [17,18], its role in DMTJ remains an unexplored area thus far.

In this Letter, we present exact model calculations of the spin-dependent resonant tunneling in double MTJ to study for the first time the effect of magnetic and non-magnetic impurities in the magnetic middle layer on the TMR, spin polarization (SP), and local current for small external bias. This approach conserves the continuity of the current in contrast to Ref. [9]. We show that the impurities may induce a shift of the original QWS depending on the sign of the impurity scattering potential, the impurity position, and the symmetry of the original QWS. These effects can tune selectively the spin channels, giving rise to a wide variety of novel and interesting

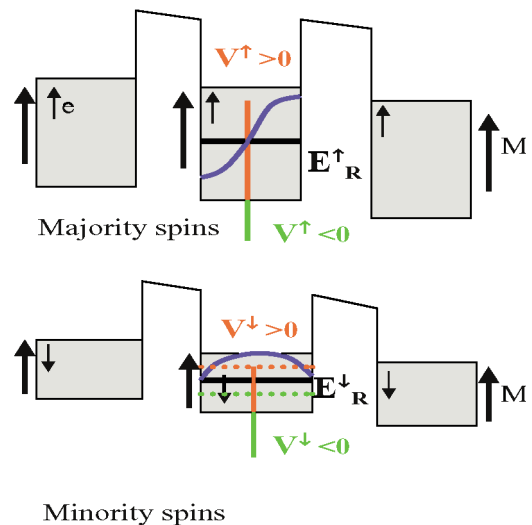


FIG. 1 (color). Schematic energy diagram for the FM configuration for the majority and the minority spin carriers. The QWS energies E_R^{σ} fall within the majority (minority) band and they are ASM (SM). The impurity δ -type potential V^{σ} of positive (negative) sign relative to the bottom of the band in the well is denoted with a red (green) line. There is no shift of the ASM QWS, whereas the SM QWS shift towards higher (lower) values if $V^{\sigma} > 0 (< 0)$.

spin-dependent transport phenomena, such as an enhancement or suppression of the TMR and the spin polarization, and a sign reversal of the SP. The calculations reveal that, even though the effect of the impurity on the average spin current is small for antisymmetric QWS, the local spin current exhibits strong variation.

We employ the free-electron band model to describe the electron tunneling in DMTJ with impurities in the metallic middle layer of width b , whose scattering is modeled by a spin-dependent δ -function scattering potential. Figure 1 shows a schematic diagram of the energy bands for the ferromagnetic (FM) configuration under a

small external bias for the majority and minority spin carriers, respectively. The geometric parameters of the DMTJ are chosen in such a way that the spin-dependent QWS energies, E_R^σ , fall within the majority (minority) spin band and they are of antisymmetric (ASM) [symmetric (SM)] character. The impurity potential V^σ relative to the bottom of the band in the middle layer is also shown with a green (red) line for positive (negative) sign, with the impurity placed at the center of the well.

Employing the WKB approximation in the barrier region, the one-electron Green's functions for the clean DMTJ are solutions of the Schrödinger equation,

$$\left[E + \frac{\hbar^2}{2m_i} \left(\frac{\partial^2}{\partial z^2} - \kappa^2 \right) - \tilde{V}_i^\sigma - ev(z) \right] G^\sigma(\kappa; z, z') = \delta(z - z'), \quad (1)$$

where $\tilde{V}_i^\sigma = V_i^\sigma$ in the metallic layers, $\tilde{V}_i^\sigma = U_i$ in the barriers, and $i = 1, \dots, 5$ refers to the i th layer. Here, V_i^σ is the spin-dependent potential (or the bottom of the band) of the i th metal, U_i is the potential barrier height in the i th barrier, and $v_i(z)$ is the voltage drop within the i th layer, assumed to be nonzero only in the barriers. The z is the coordinate perpendicular to the interface, κ is the in-plane wave vector of energy E , and m_i is the electron effective mass in the i th layer. Depending upon which layer the z and z' coordinates of the Green's function belong to, $G^\sigma(\kappa; z \in i, z' \in j) \equiv G_{ij}^\sigma(\kappa; z, z')$. The coefficients of the wave functions in each layer are determined by the boundary conditions at the interfaces.

The one-electron Green's function in the presence of the impurity is determined from the Dyson equation:

$$\tilde{G}^\sigma(\rho, z, \rho', z') = G^\sigma(\rho, z, \rho', z') + G^\sigma(\rho, z, \rho_0, z_0) T^\sigma \times G^\sigma(\rho_0, z_0, \rho', z'), \quad (2)$$

where $T^\sigma = V^\sigma [1 - V^\sigma G_{33}^\sigma(\rho_0, z_0, \rho_0, z_0)]^{-1}$ is the **T** ma-

trix, ρ is the coordinate parallel to the interface, $V^\sigma = V_{\text{imp}}^\sigma \delta(z - z_0) - V_3^\sigma$, ρ_0, z_0 is the impurity position, and G_{33}^σ is the Green's function in the metallic middle layer. Here, V^σ (V_{imp}^σ) refers to the impurity potential relative to the bottom of the band (Fermi energy, E_F) of the well. Depending on the width of the quantum well and the sign of V^σ , the poles of the **T** matrix give rise to *impurity-induced* shift of resonances, which can in turn enhance or suppress selectively the current density of the majority or minority spin channel for a given magnetization orientation.

The local current density for spin σ is given by [19]

$$j^\sigma(\rho - \rho_0, z) = \frac{e}{\pi \hbar} \int [f(E) - f(E + eV_{\text{ext}})] \times D^\sigma(E, \rho - \rho_0, z) dE, \quad (3)$$

where $f(E)$ is the Fermi-Dirac distribution function, and the transmission probability D^σ is [20]

$$D^\sigma(E, \rho - \rho_0, z) = \left(\frac{\hbar^2}{2m} \right)^2 \int d\rho' A^\sigma(E, \rho, z; \rho', z') \tilde{\nabla}_z \tilde{\nabla}_{z'} A^\sigma(E, \rho, z; \rho', z'). \quad (4)$$

Here, $\tilde{\nabla}_z = (1/2)(\tilde{\nabla}_z - \tilde{\nabla}_z)$ is the antisymmetric gradient operator, $A^\sigma(E, \rho, z; \rho', z') = (i/2)[G^{\text{ret},\sigma}(E, \rho, z; \rho', z') - G^{\text{adv},\sigma}(E, \rho, z; \rho', z')]$, where $G^{\text{ret},\sigma}$ and $G^{\text{adv},\sigma}$ are the retarded and advanced Green's functions, respectively. The total transmission probability $D = D^{(0)} + D^{(1)} + D^{(2)}$, where $D^{(0)}$ is the transmission probability in the absence of impurity, and $D^{(1)}$ and $D^{(2)}$ are proportional to the **T** matrix and to the **T** matrix squared, respectively. The average current j^σ can be calculated from Eq. (3) but with $D^\sigma(E, \rho - \rho_0, z)$ replaced with its average value

$$\langle D^\sigma(E, z) \rangle = \frac{N_{\text{imp}}}{N} \int D^\sigma(E, \rho - \rho_0, z) d\rho, \quad (5)$$

where the number of impurities $N_{\text{imp}} = cN$, c is the impurity concentration, and N is the total number of atoms in the plane. We find that the average current is independent of z , satisfying the current continuity equation.

We model an Fe/Oxide/Fe/Oxide/Fe DMTJ, with $V_1^\uparrow = V_3^\uparrow = V_5^\uparrow = -4.58$ eV and $V_1^\downarrow = V_3^\downarrow = V_5^\downarrow = -0.66$ eV [4]. The barrier widths are 8 Å and 2 Å, respectively, $c = 5\%$, and the impurity is placed at the center of the well. A more appropriate treatment for the DMTJ with $c = 5\%$ is the coherent potential approximation approach for the alloy, rather the simpler approach we used of a system of noninteracting impurities. However, the correction to our result for the average current is proportional to $cN^\sigma(E_F)V^\sigma$, where $N^\sigma(E_F)$ is the quasi-two-dimensional density of states at E_F in the middle layer. When the resonance state is within the band [$N^\sigma(E_F) \neq 0$], the product of $N^\sigma(E_F)V^\sigma \rightarrow 1$, and hence the correction, is small of the order of $c = 5\%$. Furthermore, calculations for nonmagnetic impurities and for a middle-layer thickness of 4.3 Å show that for $V_{\text{imp}} = -2(+2)$ eV the TMR is 135(152)% for $c = 0.5\%$, compared to the value of

95(380)% for $c = 5\%$ and of 142(142)% for $c = 0$. Thus, these results indicate that although the effect on the TMR is smaller for lower c , the conclusions of this work do not change.

In Fig. 2 we show the $\text{TMR} = (j_P - j_{AP})/j_{AP}$ [6] as a function of the well thickness for the perfect DMTJ and in the presence of nonmagnetic impurities with $V_{\text{imp}} = 0, +2, -2$ eV. Here, j_P (j_{AP}) is the current density in the ferromagnetic (FM) [antiferromagnetic (AFM)] configuration in which the leads are ferromagnetically (antiferromagnetically) aligned to the middle magnetic layer. The peak in the TMR at $b = 4.3$ Å for the perfect DMTJ can be dramatically enhanced (suppressed) by impurities with positive (negative) V^σ , which can shift the original QWS. For $b = 4.3$ Å, the original QWS for the majority (minority) spin for the FM (AFM) configuration are below E_F and they are ASM. On the other hand, the QWS for the minority (majority) spin for the FM (AFM) configuration are SM and above E_F . This is due to the larger (smaller) k_F^σ in the well for the majority (minority) spin band [10]. The effect of the impurity on the QWS can be understood in terms of a simple quantum mechanical model, namely, a δ -function impurity potential, V^σ , within a potential well. Symmetric QWS are shifted towards higher (lower) energies for positive (negative) impurity potential. In contrast, antisymmetric QWS are not shifted. Thus, the positive (negative) impurity potential shifts the QWS away from (closer to) E_F , suppressing (enhancing) both j_P^\uparrow and j_{AP}^\uparrow , and hence increasing (decreasing) the TMR. On the other hand, the j_P^\downarrow and j_{AP}^\downarrow are not affected by the impurity.

For $b = 7.24$ Å, in the absence of impurity the majority and minority spin QWS for both the FM and AFM

configurations are SM and below E_F . For $V_{\text{imp}} = +2, 0$ eV, both the V^\uparrow and V^\downarrow are positive and the QWS are shifted closer to E_F . Thus, the current for both FM and AFM configurations increases and the TMR decreases. For $V_{\text{imp}} = -2$ eV, the QWS for the minority (majority) spin for the FM (AFM) configuration are lowered in energy, and hence the corresponding currents decrease. On the other hand, the QWS for the majority (minority) spin for the FM (AFM) configuration are raised in energy, and hence the corresponding currents increase. However, it turns out these current components compensate each other and the TMR is not altered much.

While the issue of SP for single barriers has attracted significant interest recently, both theoretically [17,18] and experimentally [2,3], the SP in DMTJ in the presence or absence of disorder has not been addressed theoretically. The SP for the FM configuration is $\text{SP} = (j_P^\uparrow - j_P^\downarrow)/(j_P^\uparrow + j_P^\downarrow)$ [2,3]. In Fig. 3 we show the SP for the FM configuration as a function of V_{imp}^\uparrow for three values of $V_{\text{imp}}^\downarrow$ for $b = 4.3$ Å and 7.24 Å, respectively. For $b = 4.3$ Å, the SP is independent of V_{imp}^\uparrow due to the fact that the QWS for the majority spin are ASM and hence j_P^\uparrow is not affected by the impurity. On the other hand, the SP depends on $V_{\text{imp}}^\downarrow$ because the minority spin QWS are SM. In the absence of impurity, $j_P^\uparrow < j_P^\downarrow$ and hence the SP is negative. An impurity with $V_{\text{imp}}^\downarrow > 0$ decreases j_P^\downarrow and hence increases the SP, leading to a sign reversal of the SP for large enough $V_{\text{imp}}^\downarrow = 2$ eV. In contrast, j_P^\downarrow increases if $V_{\text{imp}}^\downarrow < 0$, and hence the SP decreases.

For $b = 7.24$ Å, the SP increases with increasing V_{imp}^\uparrow because the SM QWS below E_F are shifted close to E_F and j_P^\uparrow increases. Note that for $V_{\text{imp}}^\uparrow > -2$ eV the SP

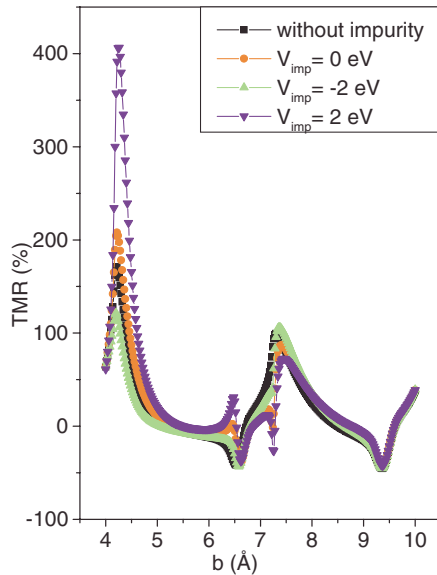


FIG. 2 (color). TMR versus the middle layer thickness b in the presence or absence of nonmagnetic impurities for different values of the impurity potential, V_{imp} .

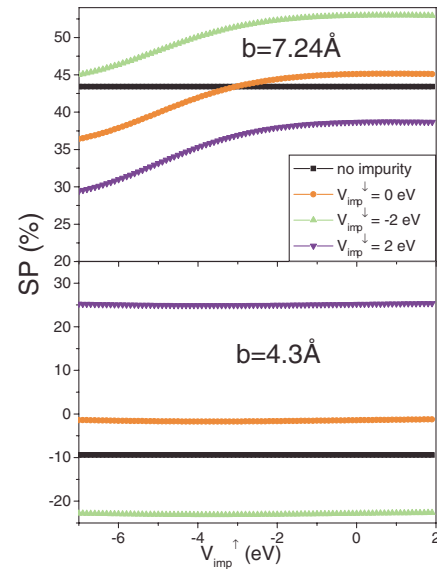


FIG. 3 (color). Spin polarization for the FM configuration as a function of V_{imp}^\uparrow in the presence or absence of impurities for different values of $V_{\text{imp}}^\downarrow$ and for $b = 4.3$ and 7.24 Å, respectively.

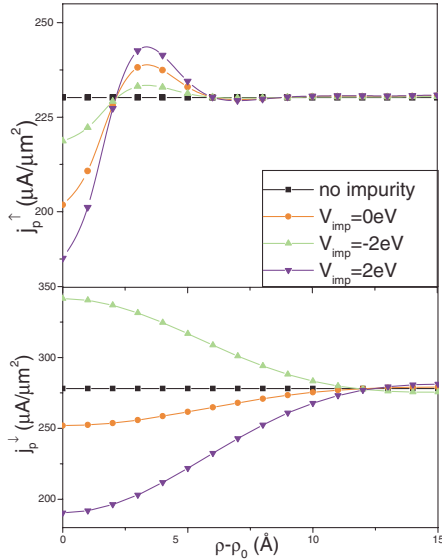


FIG. 4 (color). Local current $j_p^\sigma(\rho - \rho_0)$ in the center of the first barrier as a function of $\rho - \rho_0$ for $b = 4.3 \text{ \AA}$ and for various values of V_{imp} for the FM configuration.

varies weakly with V_{imp}^\uparrow , due to the fact that the QWS lie in an energy range within $k_B T$ around E_F . On the other hand, for $V_{\text{imp}}^\uparrow = 0$ and 2 eV , the QWS are shifted closer to E_F ($V^\uparrow > 0$), and hence j_p^\uparrow increases and the SP decreases. In contrast, for $V_{\text{imp}}^\uparrow = -2 \text{ eV}$, the QWS are shifted away from E_F ($V^\uparrow < 0$), and hence j_p^\uparrow decreases and the SP increases.

In order to understand the effect of a nonmagnetic impurity on the distribution of the local current in its vicinity, we present in Fig. 4 the local current, $j_p^\sigma(\rho - \rho_0)$, at the center of the first barrier as a function of $\rho - \rho_0$ for $b = 4.3 \text{ \AA}$ and for various values of V_{imp} for the FM configuration. Note that, while the average current for the majority spin channel is not affected by the impurity because the QWS are ASM (Fig. 2), the local current is dramatically changed compared to its corresponding value for the pure DMTJ. The effect is larger as the impurity potential increases. On the other hand, for the minority spin the local current in the vicinity of the impurity decreases for $V_{\text{imp}} = 0, +2 \text{ eV}$ and increases for $V_{\text{imp}} = -2 \text{ eV}$, consistent with the behavior of the average current behavior (Fig. 1). For distances larger than 10 \AA the electrons do not feel the impurity. These spatial fluctuations of the tunneling current (“hot spots”) can have dramatic consequences on the TMR [21].

In conclusion, we have presented exact model calculations for the effect of impurities in the well on the spin-dependent resonant tunneling for DMTJ. To the best of our knowledge, these are the first calculations to address the effect of impurity in DMTJ. The calculations reveal that the spin-dependent impurity scattering potential can tune selectively the majority and minority spin channels, giving rise to a wide variety of interesting and unusual transport phenomena. We find that the impurities can lead

to a dramatic enhancement or suppression or sign reversal of the TMR and the SP. The proposed underlying mechanism, which explains consistently the overall behavior, is the shift of the original QWS depending on (i) the SM or ASM nature of these QWS and (ii) the impurity scattering potential. Although the effect of the impurity on the average spin current is small for ASM QWS, the local spin current exhibits strong variation. The effect of impurities on the TMR with nonzero external bias will be presented in a future publication.

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