Eur. Phys. J. B **31**, 463–469 (2003)
DOI: 10.1140/epjb/e2003-00056-0

THE EUROPEAN PHYSICAL JOURNAL B

Analytical result of the effect of spin scattering and impurity-assistance on magnetoresistance in doped magnetic tunneling junctions

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Received 13 January 2002 / Received in final form 30 November 2002

Abstract. An extended tunneling Hamiltonian method is proposed to study the temperature-dependent tunneling magnetoresistance (TMR) in doped magnetic tunnel junctions. It is found that for nonmagnetic dopants (Si), impurity-assisted tunneling is mainly elastic, giving rise to a weak spin polarization, thereby reduces the overall TMR, while for magnetic ions (Ni), the collective excitation of local spins in δ-doped magnetic layer contributes to the severe drop of TMR and the behavior of the variation of TMR with temperature different from that for Si-doping. The theoretical results can reproduce the main characteristic features of experiments.

PACS. 75.70.Pa Giant magnetoresistance – 75.30.Ds Spin waves – 73.23.Hk Coulomb blockade; single-electron tunneling

1 Introduction

Ferromagnetic (FM) tunnel junctions have triggered great interest since they were shown to exhibit large tunneling magnetoresistance (TMR) [1,2]. To find the potential application of the systems to magnetic sensors and memory devices, it is important to consider the various intrinsic properties affecting magnetoresistance. It was recognized already decades ago that tunneling electrons can interact with magnetic barrier impurities [3,4], however, so far, most of theoretical and experimental works only dealt with the case of no-doping impurities inside the barrier. Impurity scattering can occur in spin-polarized transport in standard magnetic junctions, as a result, the magnetoresistance of the structure consisting of even 100% spin-polarized materials is also limited.

Experimentally, attentions are mainly focused on the resulting effect of magnetic [3] and nonmagnetic [5] impurities on the total tunnel conductance. Recently, to acquire a complete picture of spin-tunneling in the magnetic tunneling junctions, Jansen and Moodera [6] employed a controlled preparation of magnetic tunnel junctions to uniquely and directly probe the effect of impurity scattering on the conductance and tunnel electron polarization. This was done by using a δ-doped layer with a well-defined amount of foreign atoms deposited in the form of a thin sheet of submonolayer thickness in the middle of an Al_2O_3 tunnel barrier between FM electrodes Co and NiFe. They found that Si-doping produces an unpolarized, elastic contribution to the conductance, in contrast, Ni-doping exhibits a strikingly different behavior of an inverse TMR due to spin-exchange scattering.

Theoretically, a method for spin tunneling based on Schrödinger equation was applied, has been formulated by Julliere [7] and further developed by Stearns [8] and Slonczewski *et al.* [9,10]. Nevertheless, the above works all disregarded impurity scattering inside the barrier. Although Larkin *et al.* [11] applied the method to discuss the impurity scattering, they only considered nonmagnetic impurities. Also, Appelbaum [4] and Gu *et al.* [12,13] used a tunneling Hamiltonian method to account for spin tunneling.

In this paper, we extend the tunneling Hamiltonian method, in which spin collective excitation of δ-doped layer is included for Ni-dopant case, to calculate the TMR in doped magnetic tunnel junctions. It is found that, for nonmagnetic dopants (Si), impurity-assisted tunneling is weakly polarized, and reduces the whole TMR, whereas

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for magnetic dopants (Ni), the spin collective excitation in the doped magnetic layer is responsible for the much decrease of TMR and the behavior of the variation of TMR with temperature different from that of Si-doping case. The theoretical results can exhibit the main characteristic features of the experiments [6]. In the next section, we derive the tunneling model including two electron tunneling events. In Sections 3 and 4, we calculate the TMRs of Si-doping and Ni-doping, respectively. Finally, conclusions are given in Section 5.

2 Tunneling model

The structure of Si (Ni)-doping in the barrier of tunneling junction can be regarded as a double-junction system, where the δ-doping layer is corresponding to a center electrode. In fact, the doping layer is a small two-dimensional (2D) island of nanometricsize as pointed out by references [14] and [15], in which the Coulomb blockade has a significant effect on the tunneling process. The energy can be described by an effectively average level spacing $\varDelta_{\mathit{eff}}$ [14,15] due to inhomogeneous doping and it's effect on the tunneling process is included in the calculation of conductance. The island charge is quantized and the electrostatic energy E_c takes discrete values due to Coulomb blockade. The Hamiltonian of the double-junction system is

$$H = H_0 + H_T \tag{1}$$

with $H_0 = H_1 + H_2 + H_C + U$ and $H_T = H_{T_1} + H_{T_2}$, where H_C and $H_{1(2)}$ are respectively the Hamiltonians of the central electrode and the external electrodes, and

$$U = \frac{Q^2}{2C} - \frac{eV}{C}[C_1(n_{2\uparrow} + n_{2\downarrow}) + C_2(n_{1\uparrow} + n_{1\downarrow}] \tag{2}$$

with $Q = e[(n_{1\uparrow}+n_{1\downarrow})-(n_{\uparrow 2}+n_{2\downarrow})]+Q_0$, $C = C_1+C_2$, and $n_{\uparrow(\downarrow)} = n_{1\uparrow(\downarrow)} - n_{2\uparrow(\downarrow)}$ the number of excessive electrons in the central island. Here $n_{i\sigma}$ the number of electrons with spin σ that have tunneled through the ith junction, and Q_0 describes the potential difference between the central and external electrodes. The terms $H_{Ti} = H_i^+ + H_i^-$ with $H_i^- = (H_i^+)^+$ have different expressions for the following cases of Si-doping and Ni-doping. Generally, we can treat H_{Ti} as a perturbation. When the conductance G_i of each junction is smaller than quantance conductance $2e^2/\pi\hbar$, the fourth (second nonvanishing) order in H_{Ti} [16] becomes more important for the current involved in this tunneling process. The second order tunneling process is a cotunneling one or quantum macroscopic tunneling of charge, in which a charge is transfered through the island by the intermediate electron state and virtual increase of the electrostatic energy of the circuit. By using the same procedure as that in reference [16], we can obtain similar formulas of the current

$$I = e\left(\xi^{(+)} - \xi^{(-)}\right) \tag{3}$$

with

$$\begin{aligned}\xi^{(+)} = {} & \frac{2}{\hbar^4}\sum_{\substack{p,q=1,2\\ p\neq q}} \mathrm{Re}\int_{-\infty}^{t}\mathrm{d}\tau\int_{-\infty}^{\tau}\mathrm{d}\tau'\int_{-\infty}^{\tau'}\mathrm{d}\tau'' \\ & \times\left[\exp\left\{-\mathrm{i}\left[E_2(t-\tau) + eV\left(t-\tau'\right) - E_P\left(\tau'-\tau''\right)\right]/\hbar\right\}\right. \\ & \times\langle H_p^-(\tau'')H_q^-(\tau')H_1^+(t)H_2^+(\tau)\rangle \\ & - \exp\{\mathrm{i}[E_1(t-\tau) - eV(\tau-\tau') - E_p(\tau-\tau'')]/\hbar\} \\ & \left.\times\langle H_p^-(\tau'')H_q^-(\tau')H_2^+(\tau)H_1^+(t)\rangle\right]\end{aligned} \tag{4}$$

and

$$\begin{aligned}\xi^{(-)} = {} & \frac{2}{\hbar^4}\sum_{\substack{p,q=1,2\\ q\neq q}} \mathrm{Re}\int_{-\infty}^{t}\mathrm{d}\tau\int_{-\infty}^{\tau}\mathrm{d}\tau'\int_{-\infty}^{\tau'}\mathrm{d}\tau'' \\ & \times[\exp\{\mathrm{i}[E_1(t-\tau) - eV(\tau-\tau'') - E_p(\tau'-\tau'']/\hbar\} \\ & \times\langle H_2^+(\tau)H_1^+(t)H_p^-(\tau')H_q^-(\tau'')\rangle \\ & - \exp\{-\mathrm{i}[E_2(t-\tau) + eV(t-\tau'') + E_p(\tau'-\tau'']/\hbar\} \\ & \times\langle H_1^+(t)H_2^+(\tau)H_p^-(\tau')H_q^-(\tau'')\rangle],\end{aligned} \tag{5}$$

where E_i, includes $E_{i0\sigma} = U(n_{i\sigma}+1) - U(n_{i\sigma})$ due to Coulomb blockade and the energy E_{q_i} of spin collective excitation in the Ni-doped layer which will be given in Section 4. According to equation (2), we can easily obtain $E_{i0\sigma}$, namely,

$$E_{10\sigma} = \frac{e^2}{C}\left(n_\uparrow + n_\downarrow + \frac{Q_0}{e}\right) - \frac{V(C+C_2-C_1)}{2e} + E_{\sigma\sigma'} \tag{6}$$

and

$$E_{20\sigma} = \frac{e^2}{C}\left(-n_\uparrow - n_\downarrow - \frac{Q_0}{e}\right) - \frac{V(C-C_2+C_1)}{2e} + E_{\sigma\overline{\sigma'}} \tag{7}$$

with $E_{\sigma\sigma'} = \varDelta_{\mathit{eff}} + e^2/2C$ or $e^2/2C$, where σ and σ' are the spins of tunneling and excess electrons in the island, respectively, and $\overline{\sigma'}$ is the spin opposite to σ'. When the directions of σ and σ' are the same, $E_{\sigma\sigma'}$ is taken as $\varDelta_{\mathit{eff}} + e^2/2C$, otherwise, $e^2/2C$. Here we consider that the tunneling and excessive electrons with the same spins are forbidden to stay in the same energy level. As $\varDelta_{\mathit{eff}}$ is comparable with $e^2/2C$ in our system, the role of $\varDelta_{\mathit{eff}}$ becomes very important, which will be shown in the following parts.

3 Si-doping

First, we calculate the tunneling conductance of Si-doping in the light of equations (3, 4) and (5). The tunneling Hamiltonian is

$$H_{Ti} = \sum_{\alpha\beta\sigma} T^{(i)}_{\alpha\beta\sigma} d^{+}_{\alpha\sigma} c_{\beta\sigma} + \text{h.c.}, \tag{8}$$

where $d^{+}_{\alpha\sigma}(c_{\beta\sigma})$ is spin σ electron operators of electrodes including the central electrode. For the case of Si-doping, in reference [6], it is reported that the weak temperature dependence of the TMR reduction indicates that the tunneling is mainly elastic contunneling one in nature, this implies that the same electron tunnels through both of the double junctions as has been pointed in reference [16]. Substituting equation (8) into equation (4), we can get

$$\xi^{(+)} = \frac{2\pi}{\hbar} \sum_{m,n,k,l} T^{(1)}_{km\sigma} T^{*(1)}_{lm\sigma} T^{(2)}_{nk\sigma} T^{*(2)}_{nl\sigma} f(\varepsilon_m) \times [1 - f(\varepsilon_n)] F(\varepsilon_l, \varepsilon_m, \varepsilon_n) F(\varepsilon_k, \varepsilon_m, \varepsilon_n) \sigma(\varepsilon_m - \varepsilon_n + eV) \tag{9}$$

with

$$F(\varepsilon, \varepsilon_m, \varepsilon_n) = \frac{1 - f(\varepsilon)}{E_1 + \varepsilon - \varepsilon_m} - \frac{f(\varepsilon)}{E_2 - \varepsilon + \varepsilon_n}, \tag{10}$$

where $f(\varepsilon)$ is the distribution function of the electrons in the central electrode (here and below the indices m, n denote the energy eigenstates of the external electrodes, while k, l denote those of the central electrode), and in E_i, we consider that there is only $E_{i0\sigma}$ because of the absence of spin collective excitation for Si-doping. Similarly, the backward tunneling rate $\xi^{(-)}$ can be obtained, which is given by equation (9) with $V \to -V$, $E_i \to E_i + eV$ and $\varepsilon_m \leftrightarrow \varepsilon_n$. We can obtain the conductance G^{asP} in the parallel (P) magnetization configuration between the two electrodes, in which the superscript *as* denotes impurity-assisted tunneling in the presence of nonmagnetic impurity inside the barrier

$$G^{\text{asP}} = a_1 \rho_{LM} \rho_{RM} + a_2 \rho_{Lm} \rho_{Rm} \tag{11}$$

with $a_1 = \pi e^2 |\overline{T}|^4 \rho_C (1/E_{10\uparrow} + 1/E_{20\uparrow})/\hbar$ and $a_2 = \pi e^2 |\overline{T}|^4 \rho_C (1/E_{10\downarrow} + 1/E_{20\downarrow})/\hbar$, where ρ_M and ρ_m are respectively the majority and minority densities of state (DOS) of the external electrodes, and ρ_C is the DOS of the central electrode. Here it is an adequate approximation to treat the transfer rate $T_{\alpha\beta\sigma}$ as their average $\overline{T}$ [12]. For small voltages, the average of $E_{10\sigma}$ and $E_{20\sigma}$, $E_{i0\sigma} = (E_C + \Delta_{eff})/2$ with $E_C = e^2/(C)$. In Si-doping, the Bohr radius a_B of Si about 10^2 Å [14,15] is corresponding to the dimensions of the δ-doping layer. As a result, the effective energy interval Δ_{eff} can be comparable with the characteristic charging energy E_C, which implies that the effect of Δ_{eff} should be taken into account. For the antiparallel (A) magnetization configuration, one can similarly derive the G^{asA}

$$G^{\text{asA}} = a_1 \rho_{LM} \rho_{Rm} + a_2 \rho_{Lm} \rho_{RM}. \tag{12}$$

Here it is assumed that in the excessive electrons of the island, the spins up predominate, *i.e.*, $n_\uparrow > n_\downarrow$. To simplify the expression of equations (11, 12), we assume that the two electrodes are the same, then an effective spin polarization due to Si-doping is introduced

$$P^{\text{as}} = \sqrt{\frac{\rho_M - \gamma\rho_m}{\rho_M + \gamma\rho_m}} P, \tag{13}$$

where $\gamma = a_2/a_1$ and P is the spin polarization of the external electrodes, given by $P = (\rho_M - \rho_m)/(\rho_M + \rho_m)$. As a result, G^{asP} and G^{asA} reduce to

$$G^{\text{as}} = G^{\text{as}}_0 \left(1 + P^{\text{as}2} \cos\theta\right) \tag{14}$$

with

$$G^{\text{as}}_0 = \frac{1}{2} (\rho_M + \rho_m)(a_1 \rho_M + a_2 \rho_m). \tag{15}$$

Equation (14) has the same form as that in reference [6]. Here θ is the angle between the magnetization vectors of the two external electrodes and equals to 0 (π) for the P(A) magnetization configuration. After expressing equations (11, 12) as equation (14), we can easily obtain equations (13, 15). The whole tunneling conductance is $G = G_t + G^{\text{as}}$ with

$$G_t = G_0 [1 + \kappa + (1 - \kappa) P_L P_R \cos\theta], \tag{16}$$

where G_t describes the process of *direct* tunneling including *spin-conservation* and *spin-flip* for the ordinary ferromagnetic tunnel junctions [12,13] and is controlled by the constant prefactor G_0 and κ characters the spin flip effect [12]. Since $n_\uparrow > n_\downarrow$, it is concluded that from equations (6, 7), $E_{10\uparrow} > E_{10\downarrow} > 0$, $E_{20\uparrow} < E_{20\downarrow} < 0$, and $E_{10\uparrow} + E_{20\uparrow} = E_{10\downarrow} + E_{20\downarrow}$, leading to $\gamma > 1$, thus P^{as} is always smaller than P, this implies that Si-doping produces a weak spin-polarization, which is consistent with that in reference [6].

Next, in order to obtain the temperature dependence of the spin-polarization parameter P in the external electrodes, one needs to have the electron magnetization $M(T)$ as a function of temperature, which can be described by reference [17] at smaller temperatures relative to Curie' temperature T_f,

$$M(T) = M_s \left[1 - \mu \left(\frac{T}{T_f}\right)^{3/2}\right], \tag{17}$$

where μ is a constant determined by concrete magnetic material and M_s is the saturate magnetization. Then the

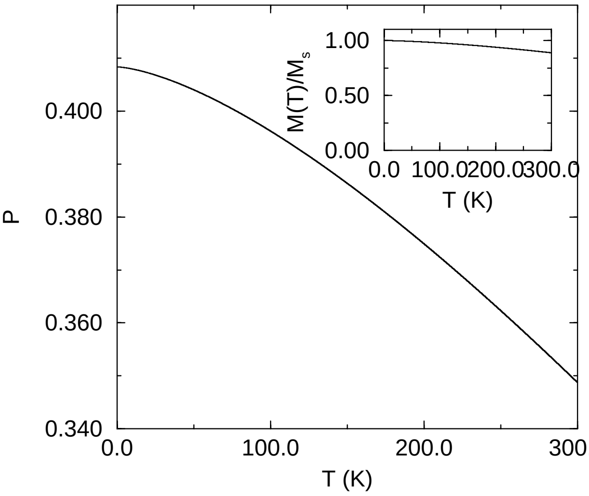

Fig. 1. Electronic spin polarization P *versus* temperature in the external electrodes. $M(T)/M_s$ *versus* temperature shown in the inset. $\mu = 0.3$, $T_f = 580$ K, and $\mu_B \lambda M_s/E_F = 0.7$.

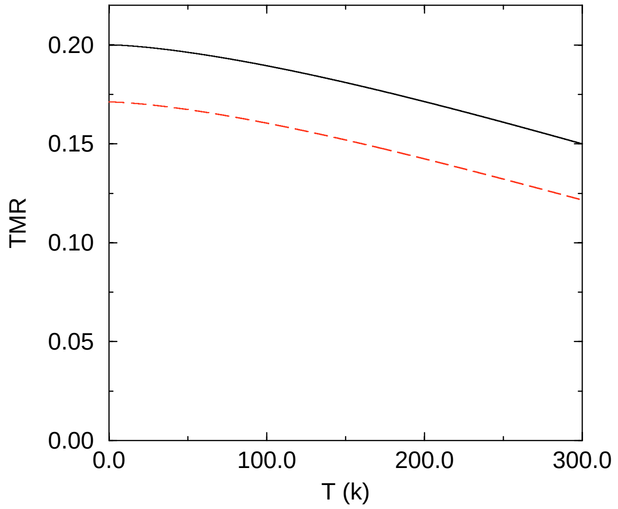

Fig. 2. Calculated TMR ratios *versus* temperature for the control case (solid line) and the Si-doping (dotted line). The parameters are taken to be $\nu = 0.5$ at zero temperature, $\kappa = 0.2$, and $\gamma = 1.5$ respectively.

DOS $\rho_{M(m)}$ of the two external electrodes can be obtained as

$$\rho_{M(m)} = \frac{4\pi V_0 (2m)^{3/2}}{h^3} \left(E_F \pm \frac{\Delta_{spl}}{2} \right)^{1/2} \tag{18}$$

with $\Delta_{spl} = \mu_B \lambda M(T)$. Here E_F is the Fermi energy, Δ_{spl} is spin splitting energy, μ_B is Bohr magneton, and λ is a constant. Although equation (18) the assumption taken from reference [13] is coarse, it does not have a significant effect on the conclusion as was done in reference [13]. In the light of equations (17, 18), the temperature dependence of the $M(T)/M_s$ and the spin polarization P in the external electrodes are shown in Figure 1. In the numerical calculation, for simplicity, the external electrodes are assumed to be the same. We take $\mu_B \lambda M_s/E_F = 0.7$, which is close to that of reference [18]. The parameters T_f and μ are respectively taken to be 580 K and 0.3. Figure 1 shows that the spin polarization slowly decreases with increasing temperature. TMR is generally defined by as $(G_P - G_{AP})/G_P$. Here the overall TMR is determined by the relative weight of conductance due to direct, impurity-assisted, and spin-exchange tunneling. For the case of Si-doping, the spin-exchange tunneling does not appear. The general expression of TMR is easily deduced from equations (14) and (16).

$$TMR = \frac{2\left[(1-\kappa)P_L P_R + \nu {P^{\mathrm{as}}}^2\right]}{1 + P_L P_R + \kappa(1 - P_L P_R) + \nu\left(1 + {P^{\mathrm{as}}}^2\right)}, \tag{19}$$

where $\nu = G_0^{\mathrm{as}}/G_0$, in which the weights of G_t and G^{as} are included. When $\nu = 0$, equation (19) reduces to

$$TMR = \frac{2(1-\kappa)P_L P_R}{1 + P_L P_R + \kappa(1 - P_L P_R)}, \tag{20}$$

which is just that of the undoped control junction [12]. Since $P^{\mathrm{as}} < P$, one can easily find from equation (19) that the TMR of the doped junction is smaller than that of the undoped control junction.

Combining equations (13, 17, 18) and (19), we give the variation of the TMR with increasing of temperature for the cases of the undoped control junction and Si-doping junction in Figure 2. Here κ charactering the spin-flip effect is taken to be 0.2, which is close to that of references [12] and [13] because the effect is always smaller compared with that of spin-conservation. γ is chosen as 1.5 according to the parameters E_C and Δ_{eff} in references [14] and [15]. We take the ratio $\nu = 0.5$ at *zero* temperature, which is reasonable. This is because the weight of impurity tunneling is smaller than that of the direct due to the small size of the 2D island. Figure 2 shows that the behavior of TMR *versus* T for Si-doping is similar to that of the undoped control junction, while the value at the same temperature is reduced. The results are in agreement with the experimental ones [6].

4 Ni-doping

To explain the *zero-bias anomaly*, the spin collective excitations localized at the interfaces between the insulating barrier and the ferromagnetic electrodes have been introduced in the tunneling theory of ferromagnetic tunnel junctions, such as Co/Al$_2$O$_3$/CoFe, using the spin-wave approximation within the framework of the transfer Hamiltonian method [19]. For Ni-doping, the central electrode is corresponding to a magnetic layer. Here, we only consider the spin collective excitation localized at the interfaces between the insulating barrier and the doped layer to stress the role of Ni-doping.

In the tunneling process of Ni-doping, there are two cases, one is that the same electron tunnels through the double tunnel junctions, only including one spin-flip event, the other is the different behaviors of two electrons, involving two spin-flip events. The tunneling Hamiltonians, which are connected with spin-exchange scattering in the barrier [4], are

$$H_{Ti} = \frac{1}{\sqrt{N}_s} \sum_{\mathbf{kpq}} \left[T^{(i)}_{\mathbf{kpq}} S^z(\mathbf{q}) \left(d^+_{k\uparrow} c_{p\uparrow} - d^+_{k\downarrow} c_{p\downarrow} \right) + \text{h.c.} \right] + \frac{1}{\sqrt{N}_s} \sum_{\mathbf{kpq}} \left[T^{(i)}_{\mathbf{kpq}} S^+(\mathbf{q}) \left(d^+_{k\downarrow} c_{p\uparrow} + c^+_{p\downarrow} d_{k\uparrow} \right) + \text{h.c.} \right]. \tag{21}$$

Here $d_{\mathbf{k}\sigma}(c_{\mathbf{p}\sigma})$ is the spin σ electron operator of the electrodes including the central electrode, $S^z_\alpha(\mathbf{q}) = (1/\sqrt{N}_s) \sum_{j\in I} S^z_{\alpha j} \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\alpha j})$ and $S^\pm_\alpha(\mathbf{q}) = (1/\sqrt{N}_s) \times \sum_{j\in I} S^\pm_{\alpha j} \exp(\pm\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\alpha j})$ with $S^\pm_{\alpha j} = (S^x_{\alpha j} \pm \mathrm{i}S^y_{\alpha j})/2$, $\alpha = L$ or R, N_s is the number of the local spins at the interface between the insulating layer and the doped layer, and $\mathbf{q}$ is the two-dimensional wave vector parallel to the interface. The Hamiltonian means the spin-flip tunneling induced by the collective excitation of the local spins at the interface, thus the electron tunneling involves the emission or absorption of the local spin collective excitation.

First, according to equation (4), we calculate the tunneling conductance of the case involving one spin-flip events, which means spin-flip in the *whole* tunneling process. The tunneling Hamiltonian H_T in the whole process is determined by equations (8) and (21). In the following parts of the paper, we use subscript *ex* to represent the tunnel process associated with spin-exchange scattering in the barrier, and superscripts *sf* and *nsf* to stand for *spin-flip* and *no spin-flip* in the *whole* tunneling process, respectively. As in Si-doping, we can obtain the conductance G^{sfP}_{ex1} for the P configuration in which E_1 and E_2 contain the spin collective excitation,

$$G^{\text{sfP}}_{ex1} = a^{\text{sf1}}_1 \rho_{LM} \rho_{Rm} + a^{\text{sf1}}_2 \rho_{Lm} \rho_{RM}, \tag{22}$$

where

$$a^{\text{sf1}}_1 = \pi e^2 T^{(1)}_{km} T^{*(1)}_{lm} T^{(2)}_{nk} T^{*(2)}_{nl} \times \varDelta_{\mathit{eff}} \left(x_{1\uparrow} \rho_{CM} \rho_{Cm} + x_{2\uparrow} \rho_{Cm} \rho_{Cm} \right) / \hbar \tag{23}$$

and

$$a^{\text{sf1}}_2 = \pi e^2 T^{(1)}_{km} T^{*(1)}_{lm} T^{(2)}_{nk} T^{*(2)}_{nl} \times \varDelta_{\mathit{eff}} \left(x_{1\downarrow} \rho_{Cm} \rho_{Cm} + x_{2\downarrow} \rho_{Cm} \rho_{CM} \right) / \hbar \tag{24}$$

with

$$x_{1\sigma} = \sum_{q_1, q_2} \left(\frac{\langle S^z(q_1) S^z(q_1) \rangle}{E_{10\overline{\sigma}}} + \frac{1}{E_{20\overline{\sigma}}} \right) \tag{25}$$

and

$$x_{2\sigma} = \sum_{q_1, q_2} \left(\frac{\langle S^-(q_1) S^+(q_1) \rangle}{E_{q_1} + E_{10\overline{\sigma}}} + \frac{1}{E_{20\overline{\sigma}}} \right) \cdot \tag{26}$$

Here the subscript $\overline{\sigma}$ means that for the electron of spin σ tunneling from one external electrode to the central island, spin-flip is caused by the collective excitation of spin, the terms ρ_{CM} and ρ_{Cm} are respectively the minority and majority DOS of the central electrode, and $E_q = D_s q^2 + E_0$ denotes the collective excitation spectrum of local spins for two-dimensional Heisenberg ferromagnet [20] with D_s the spin stiffness and E_0 the spin gap due to anisotropy in the δ-doped layer with $D_s = D\langle S^z \rangle$ in the long-wave length limit. At low temperatures, we have $\langle S^z \rangle = S$ and $D_s = DS$ [13]. It is well known that transverse correlation function is given by $\langle S^-_\alpha(q) S^+_\alpha(q) \rangle = 2\langle S^z_\alpha \rangle (\exp^{E_q/k_B T} - 1)^{-1}$. For the longitudinal correlation function, we can use a simple approximation, given by $\langle S^z_\alpha(q) S^z_\alpha(q) \rangle \approx \langle S^z_\alpha \rangle^2$. Here due to the *upward* magnetization direction of Ni-doping layer, in the excessive electrons, spins up predominate more than those in Si-doping. In addition, the effective energy interval $\varDelta_{\mathit{eff}}$ is slightly smaller that in Si-doping, however, the charging energy E_C is bigger. The conductance G^{sfA}_{ex1} in the A configuration can be similarly derived. By introducing an effective spin polarization in the same way as that in Si-doping with $\gamma^{\text{sf1}} = a^{\text{sf1}}_2 / a^{\text{sf1}}_1$, G^{sfP}_{ex1} and G^{sfA}_{ex1} reduce to

$$G^{\text{sf}}_{ex1} = G^{\text{sf1}}_0 (1 - P^{\text{sf1}^2} \cos\theta), \tag{27}$$

where G^{sf1}_0 and P^{sf1} have the same expressions as G^{as}_0 and P^{as} in Si-doping.

Next, using equations (3, 4) and (5), we calculate the tunneling conductance of the case including two spin-flip events, in which the tunneling Hamiltonian H_T in the *whole* process is only determined by equation (21). This case is further classified into two kind of cases.

(1) The directions of spins of the two excessive electrons in the doped layer are the same, which denotes spin-conserved in the *whole* tunneling process. Similarly, using the same way as that in Si-doping, the conductance G^{nsfP}_{ex} and G^{nsfA}_{ex} can be transformed into

$$G^{\text{nsf}}_{ex} = G^{\text{nsf}}_0 \left(1 + P^{\text{nsf}^2} \cos\theta \right), \tag{28}$$

where P^{nsf} and G^{nsf}_0 also have the same expressions as those in Si-doping. In P^{nsf}, $\gamma^{\text{nsf}} = a^{\text{nsf}}_2 / a^{\text{nsf}}_1$ with

$$a^{\text{nsf}}_1 = \left[\chi^+_0 \left(\chi^+_{1\uparrow} + \chi^+_{2\uparrow} \right) - \chi^-_0 \left(\chi^-_{1\uparrow} + \chi^-_{2\uparrow} \right) \right] \rho_{CM} \rho_{Cm} \tag{29}$$

and

$$a^{\text{nsf}}_2 = \left[\chi^+_0 \left(\chi^+_{1\downarrow} + \chi^+_{2\downarrow} \right) - \chi^-_0 \left(\chi^-_{1\downarrow} + \chi^-_{2\downarrow} \right) \right] \rho_{CM} \rho_{Cm}. \tag{30}$$

$$TMR = \frac{2\left[(1-\kappa)P^2 - \eta_1 {P^{\mathrm{sf1}}}^2 - \eta_2 {P^{\mathrm{sf2}}}^2 + \eta_3 {P^{\mathrm{nsf}}}^2\right]}{1 + P^2 + \kappa\left(1-P^2\right) + \eta_1\left(1-{P^{\mathrm{sf1}}}^2\right) + \eta_2\left(1-{P^{\mathrm{sf2}}}^2\right) + \eta_3\left(1+{P^{\mathrm{nsf}}}^2\right)}, \tag{38}$$

Here

$$\chi_0^+ = \frac{2\pi e^2}{\hbar}\left|T_{km}^{(1)}\right|^2\left|T_{nl}^{(2)}\right|^2\left\{\frac{1}{6}(eV)^2 + \frac{2}{3}(\pi k_B T)^2\right\} \times \left[1 - \exp^{-eV/(k_B T)}\right]^{-1}, \tag{31}$$

$$\chi_{1\sigma}^+ = \sum_{q_1,q_2} \frac{1}{N_s^2}\left(\frac{\langle S^z(q_1)S^z(q_1)\rangle}{E_{10\overline{\sigma}}} + \frac{\langle S^z(q_2)S^z(q_2)\rangle}{E_{20\overline{\sigma}}}\right)^2, \tag{32}$$

$$\chi_{2\sigma}^+ = \sum_{q_1,q_2} \frac{1}{N_s^2}\left(\frac{\langle S^-(q_1)S^+(q_1)\rangle}{E(q_1) + E_{10\overline{\sigma}}} + \frac{\langle S^-(q_2)S^+(q_2)\rangle}{E(q_2) + E_{20\overline{\sigma}}}\right)^2, \tag{33}$$

χ_0^-, $\chi_{1\sigma}^-$ and $\chi_{2\sigma}^-$ are obtained respectively through χ_0^+, $\chi_{1\sigma}^+$ and $\chi_{2\sigma}^+$ with $V \to -V$ and $E_q \to E_q + eV$.

(2) The directions of spins of the two excessive electrons in the doped layer are different, this implies spin-flip in the *whole* tunneling process. The conductance is deduced as

$$G_{ex2}^{\mathrm{sf}} = G_0^{\mathrm{sf2}}(1 - {P^{\mathrm{sf2}}}^2 \cos\theta), \tag{34}$$

where similarly, G_0^{sf2} and P^{sf2} have the same expressions as those in Si-doping. In P^{sf2}, $\gamma^{\mathrm{sf2}} = a_2^{\mathrm{sf2}}/a_1^{\mathrm{sf1}}$ with

$$a_1^{\mathrm{sf2}} = \left(\chi_0^+\chi_{1\uparrow}'^+ - \chi_0^-\chi_{1\uparrow}'^-\right)\rho_{CM}^2 + \left(\chi_0^+\chi_{2\uparrow}'^+ - \chi_0^-\chi_{2\uparrow}'^-\right)\rho_{Cm}^2 \tag{35}$$

and

$$a_2^{\mathrm{sf2}} = \left(\chi_0^+\chi_{1\downarrow}'^+ - \chi_0^-\chi_{1\downarrow}'^-\right)\rho_{Cm}^2 + \left(\chi_0^+\chi_{2\downarrow}'^+ - \chi_0^-\chi_{2\downarrow}'^-\right)\rho_{CM}^2. \tag{36}$$

Here the terms $\chi_{1\sigma}'^+$ and $\chi_{1\sigma}'^+$ are determined by equations (32, 33) with $E_{20\overline{\sigma}} \to E_{20\sigma}$, $\chi_{1\sigma}'^-$ and $\chi_{2\sigma}'^-$ are obtained respectively through $\chi_{1\sigma}'^+$ and $\chi_{2\sigma}'^+$ with $V \to -V$ and $E_q \to E_q + eV$. Therefore, the overall conductance can be expressed by $G = G_t + G_{ex}$, where

$$G_{ex} = G_{ex}^{\mathrm{nsf}} + G_{ex}^{\mathrm{sf}} = G_0^{\mathrm{nsf}}(1 + {P^{\mathrm{nsf}}}^2\cos\theta) + G_0^{\mathrm{sf1}}(1 - {P^{\mathrm{sf1}}}^2\cos\theta) + G_0^{\mathrm{sf2}}(1 - {P^{\mathrm{sf2}}}^2\cos\theta). \tag{37}$$

It is found that equation (37) has the similar form with that in reference [6]. The difference is that the spin polarization P in reference [6] is replaced by P^{sf1}, P^{sf2} and P^{nsf}, respectively. equations (14) and (37) are the main results in this paper. Finally, the TMR can be obtained

see equation (38) above,

where $\eta_1 = G_0^{\mathrm{sf1}}/G_0$, $\eta_2 = G_0^{\mathrm{sf2}}/G_0$, and $\eta_3 = G_0^{\mathrm{nsf}}/G_0$. Here the weight of the first case included in η_1 and the sum of the two equal weights of the second case included in η_2 and η_3 have been assumed to be the same. Obviously, η_1 and η_2, the spin-flip terms, give an inverse contribution to the TMR, in addition, η_1, η_2 and η_3 vary with increasing temperature, which result in that the variation of the TMR with temperature in the doped junction is different from that in the undoped. Combining equations (18, 27, 28, 34), and (38), we can obtain the variation of the TMR as a function of temperature in Figure 3. The material parameters $D = 320$ meV Å^2 and $E_0 = 0.35$ meV used in numerical calculation are respectively taken to be their measured values [15,20,21]. In addition, in the light of the parameters E_C and $\varDelta_{eff}$ in references [14] and [15], $E_{10\uparrow}$, $E_{10\downarrow}$, $E_{20\uparrow}$, and $E_{20\downarrow}$, are taken to be 2.3, 1.38, −1.84 and −0.92 meV, respectively. Generally, ρ_{CM} and ρ_{Cm} of the 2D island hardly have no change with temperature. η_1 at *zero* temperature is taken to be 0.25, which is also rational and has the same reason as that for Si-doping. We have chosen $\rho_{CM}/\rho_{Cm} = 2$ [19]. It is found that the TMR has a severe drop and goes up significantly faster than that for the control junctions, which are consistent with the experimental results [6]. In addition, we find the variation of the ratio of magnetic to Fermi energy does not exhibit an important effect on the conclusion both for Si-doping and Ni-doping.

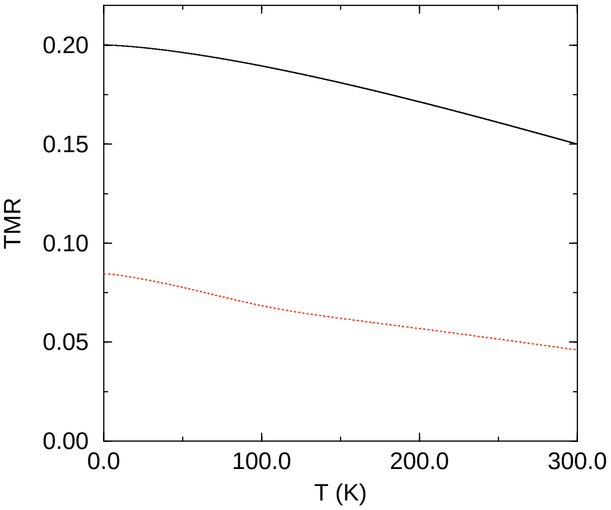

Fig. 3. Calculated TMR ratios *versus* temperature for the control (solid line) and Ni-doping cases (dotted line). Here $D = 320$ meV Å^2, $E_0 = 0.35$ meV, $\rho_{CM}/\rho_{Cm} = 2.$, and $\eta_1 = 0.25$ at *zero* temperature. $E_{10\uparrow}$, $E_{10\downarrow}$, $E_{20\uparrow}$, and $E_{20\downarrow}$, are taken to be 2.3, 1.38, −1.84 and −0.92 meV, respectively. The other parameters are the same as those in Figure 2.

5 Conclusion

We have proposed the mechanism of the temperature-dependent tunneling magnetoresistance (TMR) in doped magnetic tunnel junctions. Using an extended transfer Hamiltonian method, we show that for Si-doping, impurity-assisted tunneling is mainly elastic, giving rise to a weak spin polarization, thus reduces the overall TMR, while for magnetic ions (Ni), the collective excitation in δ-doped magnetic layer plays an important role in the much decrease of the TMR and the different behavior of the variation of the TMR with temperature. The theoretical results are consistent with those of the experiments.

This work was supported by the National Science Foundation.

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