

Magnetoresistance for the ferromagnetic tunnel junction with an amorphous semiconducting barrier

Ming-wen Xiao, Zheng-zhong Li, and Wang Xu

Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China

(Received 30 November 2002; revised manuscript received 28 January 2003; published 14 May 2003)

Considering the influences of the phonons and localized defect states in the amorphous-semiconducting barrier of a ferromagnetic tunnel junction, we have developed a tunneling theory of the interlayer exchange coupling for such a heterostructure. In this paper, we will extend our previous works to study the magnetoconductance of the junction. It is found that the magnetoconductance difference between the parallel and antiparallel spin arrangements of the electrodes can oscillate with the increase of the barrier thickness and can be enhanced by the elevation of temperature, which arise physically from the spin-flip scattering of the tunneling electrons with the localized defect states in the amorphous barrier and the interaction of the tunneling electrons with the phonons, respectively. We believe that this theoretical prediction could be observed in future experiments.

DOI: 10.1103/PhysRevB.67.195316

PACS number(s): 75.70.Cn, 72.10.Fk, 72.10.Di

The magnetoresistance (MR) in ferromagnetic tunnel junctions, first observed more than two decades ago,^{1,2} has become of fundamental interest recently because it is potentially applicable to magnetic sensors and memory devices.³ Among various junctions, the one with an amorphous-semiconducting barrier⁴⁻¹¹ distinguishes itself from the others by the well-known fact that there exists, as a characteristic, a large number of disordered localized states in an amorphous semiconductor. To understand the properties of this kind of junction theoretically, it is important to take into account the influence of these localized states. Following this idea, we have developed a tunneling theory for the exchange coupling between two ferromagnets separated by an amorphous-semiconducting barrier.^{12,13} Within the framework of this theory, there exist direct non-spin-flip tunneling, assisted spin-flip tunneling, and assisted non-spin-flip tunneling, that are in favor of long-range ferromagnetic coupling, middle-range antiferromagnetic coupling, and short-range ferromagnetic coupling, respectively. Here, the two assisted tunnelings arise from the scattering between the tunneling electrons and the disordered localized states in the amorphous barrier when the electrons tunnel through the barrier. The interlayer exchange coupling will oscillate from a ferromagnetic type to an antiferromagnetic one and back to a ferromagnetic one with the increase of the barrier thickness if the spin-flip tunneling is strong enough. Otherwise, the coupling is always ferromagnetic. At finite temperatures, after incorporating the effect of phonons into this theory, the interlayer exchange coupling becomes heat activated.¹³ Those results are in good agreement with the experiments.⁴⁻¹¹ It thus encourages us to study the effect of the localized states on the MR occurring in the ferromagnetic tunnel junction with an amorphous-semiconducting barrier in this paper, although there have been no experimental reports on this point as yet, to our knowledge.

Magnetoresistance is a relative change in a junction conductance with respect to the change of mutual orientation of spins from parallel to antiparallel, it has two definitions in the literature:¹⁴ the Jullière's tunnel-junction magnetoresistance (JMR) and the tunnel magnetoresistance (TMR),

$$J \equiv \frac{G_P - G_A}{G_P}, \quad (1)$$

$$T \equiv \frac{G_P - G_A}{G_A}, \quad (2)$$

where G_P and G_A are the conductances with the magnetizations of the two ferromagnetic electrodes parallel and antiparallel, respectively. From the two definitions of Eqs. (1) and (2), one sees that the difference between the conductances of parallel and antiparallel configurations plays the central role in the study of the MR,

$$\Delta G = G_P - G_A, \quad (3)$$

the G_P or G_A used just as a comparison factor. For this reason, we would rather study ΔG than the JMR or TMR in this paper, and from now on we shall call ΔG magnetoconductance-difference for convenience.

According to Ref. 12, the Hamiltonian of the system considered can be derived from

$$H = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \left[-\frac{1}{2m} \nabla^2 + u(\mathbf{r}) \right] \psi(\mathbf{r}) + \frac{1}{2} \int \int d\mathbf{r}_1 d\mathbf{r}_2 \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) v(\mathbf{r}_1 - \mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1), \quad (4)$$

where m represents the electron mass, $u(\mathbf{r})$ the single-electron potential, $v(\mathbf{r}_1 - \mathbf{r}_2)$ the Coulomb interaction between two electrons, and $\psi(\mathbf{r})$ the electron-field operator which can be represented by

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}, \sigma} d_{\mathbf{k}, \sigma} \phi_{l\mathbf{k}}(\mathbf{r}) \eta_\sigma + \sum_{\mathbf{q}, \sigma} f_{\mathbf{q}, \sigma} \phi_{r\mathbf{q}}(\mathbf{r}) \eta_\sigma + \sum_{i, \sigma} c_{i, \sigma} w(\mathbf{r} - \mathbf{R}_i) \eta_\sigma, \quad (5)$$

where η_σ denotes the spin wave function, $\phi_{l\mathbf{k}}(\mathbf{r})$, $\phi_{r\mathbf{q}}(\mathbf{r})$, and $w(\mathbf{r} - \mathbf{R}_i)$ are the wave functions of the left electrode,

right electrode, and the localized defect states in the amorphous barrier, respectively, and $d_{\mathbf{k},\sigma}$, $f_{\mathbf{q},\sigma}$, and $c_{i,\sigma}$ are the corresponding annihilation operators.

At finite temperatures, one should consider the effect of phonons on the electronic states, which can be incorporated by the single-electron potential, $u(\mathbf{r})$, and the localized states in the amorphous barrier, $w(\mathbf{r}-\mathbf{R}_i)$,

$$u(\mathbf{r}) = \sum_i \mathcal{V}(\mathbf{r}-\mathbf{R}_i) = \sum_i \mathcal{V}(\mathbf{r}-\mathbf{R}_i^{(0)}-\mathbf{x}_i), \quad (6)$$

$$w(\mathbf{r}-\mathbf{R}_i) = w(\mathbf{r}-\mathbf{R}_i^{(0)}-\mathbf{x}_i), \quad (7)$$

where $\mathcal{V}(\mathbf{r}-\mathbf{R}_i)$ represents the contribution to $u(\mathbf{r})$ from the i th atom, $\mathbf{R}_i^{(0)}$ denotes the equilibrium position of the i th atom, \mathbf{x}_i the deviation of the i th atom from its equilibrium position, and $\mathbf{R}_i = \mathbf{R}_i^{(0)} + \mathbf{x}_i$ the instantaneous position of the i th atom. Obviously, \mathbf{x}_i describes the vibration of the i th atom, in the continuum limit, it can be represented by phonon operators as follows:

$$\mathbf{x}_i = \sum_{\mathbf{p},\lambda} \mathbf{e}_{\mathbf{p},\lambda} \frac{1}{\sqrt{2\rho V \omega_{\mathbf{p},\lambda}}} D_{\mathbf{p},\lambda} e^{i\mathbf{p}\cdot\mathbf{R}_i^{(0)}}, \quad (8)$$

where $\mathbf{e}_{\mathbf{p},\lambda}$ stands for the polarization vector, ρ the mass density of the system, V the volume, $\omega_{\mathbf{p},\lambda}$ the phonon frequency, and $D_{\mathbf{p},\lambda} = a_{\mathbf{p},\lambda} + a_{-\mathbf{p},\lambda}^\dagger$, with $a_{\mathbf{p},\lambda}$ being the phonon annihilation operator. Expanding $u(\mathbf{r})$ and $w(\mathbf{r}-\mathbf{R}_i)$ to the linear term of $D_{\mathbf{p},\lambda}$ and substituting Eqs. (5)–(8) into Eq. (4), we obtain the working Hamiltonian,

$$H = H_0 + H' = H_0 + H_1 + H_2 + H_3 + H_4 + H_5 + H_6, \quad (9)$$

with

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma} + \sum_{\mathbf{q},s} \zeta_{\mathbf{q},s} f_{\mathbf{q},s}^\dagger f_{\mathbf{q},s} + \sum_{\mathbf{p},\lambda} \omega_{\mathbf{p},\lambda} \left(a_{\mathbf{p},\lambda}^\dagger a_{\mathbf{p},\lambda} + \frac{1}{2} \right), \quad (10)$$

$$H_1 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,s} [T_{\mathbf{k},\mathbf{q}}^{(1)} U_{\sigma s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} + \text{H.c.}], \quad (11)$$

$$H_2 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,\nu,s} \sum_i [T_{i,\mathbf{k},\mathbf{q}}^{(2)} \mathbf{S}_i \cdot \vec{\tau}_{\sigma\nu} U_{\nu s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} + \text{H.c.}], \quad (12)$$

$$H_3 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,s} \sum_{i \neq j} [T_{i,j,\mathbf{k},\mathbf{q}}^{(3)} U_{\sigma s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} + \text{H.c.}], \quad (13)$$

$$H_4 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,s} \sum_{\mathbf{p},\lambda} \sqrt{\omega_{\mathbf{p},\lambda}} [T_{\mathbf{k},\mathbf{q},\mathbf{p}}^{(4)} U_{\sigma s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} D_{\mathbf{p},\lambda} + \text{H.c.}], \quad (14)$$

$$H_5 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,\nu,s} \sum_i \sum_{\mathbf{p},\lambda} \sqrt{\omega_{\mathbf{p},\lambda}} [T_{i,\mathbf{k},\mathbf{q},\mathbf{p}}^{(5)} \mathbf{S}_i \cdot \vec{\tau}_{\sigma\nu} \times U_{\nu s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} D_{\mathbf{p},\lambda} + \text{H.c.}], \quad (15)$$

$$H_6 = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,s} \sum_{i \neq j} \sum_{\mathbf{p},\lambda} \sqrt{\omega_{\mathbf{p},\lambda}} \times [T_{i,j,\mathbf{k},\mathbf{q},\mathbf{p}}^{(6)} U_{\sigma s}(\theta) d_{\mathbf{k},\sigma}^\dagger f_{\mathbf{q},s} D_{\mathbf{p},\lambda} + \text{H.c.}], \quad (16)$$

where, according to Ref. 13, we only retain H_0 to H_6 . Here, H_0 represents the energies of the electrons on the left and right ferromagnetic (FM) electrodes and the energy of the free phonons, the two FM electrodes have the magnetic quantization axis of itself, and differ from each other by an angle θ ; H_1 to H_6 represent the tunneling Hamiltonians, and $T_{\mathbf{k},\mathbf{q}}^{(1)}$, $T_{i,\mathbf{k},\mathbf{q}}^{(2)}$, $T_{i,j,\mathbf{k},\mathbf{q}}^{(3)}$, $T_{\mathbf{k},\mathbf{q},\mathbf{p}}^{(4)}$, $T_{i,\mathbf{k},\mathbf{q},\mathbf{p}}^{(5)}$, and $T_{i,j,\mathbf{k},\mathbf{q},\mathbf{p}}^{(6)}$ are the corresponding tunneling matrices¹²; the $\vec{\tau}$ is the Pauli matrix vector, and $U(\theta) = \exp(i\tau_y \theta)$. If the effect of the phonons is neglected, we have $H = H_0 + H_1 + H_2 + H_3$. It describes the zero-temperature case considered in Ref. 12 where H_1 represents direct non-spin-flip tunneling, H_2 the spin-flip tunneling assisted by the localized states in the barrier, and H_3 the non-spin-flip tunneling assisted by the localized states in the barrier with the effects of the localized states being renormalized and incorporated into the tunneling matrix $T_{i,j,\mathbf{k},\mathbf{q}}^{(3)}$.¹² Due to the cooperation and competition among H_1 , H_2 , and H_3 , the interlayer exchange coupling will oscillate with the increasing of the barrier thickness if the assisted spin-flip tunneling H_2 is strong enough. H_4 , H_5 , and H_6 are, respectively, the phonon modifications to H_1 , H_2 , and H_3 . They describe phonon-assisted tunnelings that have no influence at zero temperature, and thus can be omitted in the zero-temperature case.¹² After incorporating the phonon modifications into the exchange coupling, the exchange coupling exhibits a heat-activated behavior at finite temperatures.¹³ Therefore, the combination of the localized states and phonons can result in both the oscillation and heat activation of the interlayer exchange coupling. In the following, we will show that such a combination can also lead to the oscillation and heat-activation of the magnetoconductance-difference.

With the Hamiltonian of Eq. (9), the tunneling current I can be expressed as^{15,16}

$$I = -e \langle I^H(t) \rangle, \quad (17)$$

$$I^H(t) \equiv \frac{d}{dt} N_L^H(t), \quad (18)$$

where $-e$ denotes the electron charge, $\langle I^H(t) \rangle$ is the thermal average of the operator $I^H(t)$, and $N_L^H(t)$ represents the total number of the electrons in the left electrode within the Heisenberg picture:

$$N_L^H(t) = e^{iHt} \cdot N_L \cdot e^{-iHt}, \quad (19)$$

$$N_L = \sum_{\mathbf{k}, \sigma} d_{\mathbf{k}, \sigma}^\dagger d_{\mathbf{k}, \sigma}. \quad (20)$$

Equation (18) indicates that $I^H(t)$ can be given by the equation of motion of $N_L^H(t)$:

$$I^H(t) = -i[N_L^H(t), H^H(t)] = -ie^{iHt} \cdot [N_L, H'] \cdot e^{-iHt}. \quad (21)$$

For the Hamiltonian of Eq. (9), we will treat H' as a perturbation to H_0 . Therefore, the tunneling current I can be given by the linear response theory,¹⁵⁻¹⁷

$$I = -e \int_{-\infty}^{+\infty} d(t-t') \langle \langle I(t) | H'(t') \rangle \rangle, \quad (22)$$

where $\langle \langle A(t) | B(t') \rangle \rangle$ represents the retarded Green's function (GF) of $A(t)$ and $B(t')$, and $A(t)$ and $B(t')$ are the operators within the interaction picture instead of the Heisenberg picture:

$$I(t) = -ie^{iH_0 t} \cdot [N_L, H'] \cdot e^{-iH_0 t}, \quad (23)$$

$$\begin{aligned} H'(t') &= e^{iH_0 t'} \cdot H' \cdot e^{-iH_0 t'} \\ &= H_1(t') + H_2(t') + H_3(t') \\ &\quad + H_4(t') + H_5(t') + H_6(t'). \end{aligned} \quad (24)$$

Substituting N_L of Eq. (20) and H' of Eq. (9) into Eq. (23), we find

$$I(t) = I_1(t) + I_2(t) + I_3(t) + I_4(t) + I_5(t) + I_6(t), \quad (25)$$

$$I_1(t) = -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, s} [T_{\mathbf{k}, \mathbf{q}}^{(1)} U_{\sigma s}(\theta) d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) - \text{H.c.}], \quad (26)$$

$$\begin{aligned} I_2(t) &= -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, \nu, s} \sum_i [T_{i, \mathbf{k}, \mathbf{q}}^{(2)} \mathbf{S}_i \cdot \vec{\tau}_{\sigma \nu} U_{\nu s}(\theta) \\ &\quad \times d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) - \text{H.c.}], \end{aligned} \quad (27)$$

$$I_3(t) = -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, s} \sum_{i \neq j} [T_{i, j, \mathbf{k}, \mathbf{q}}^{(3)} U_{\sigma s}(\theta) d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) - \text{H.c.}], \quad (28)$$

$$\begin{aligned} I_4(t) &= -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, s} \sum_{\mathbf{p}, \lambda} \sqrt{\omega_{\mathbf{p}, \lambda}} [T_{\mathbf{k}, \mathbf{q}, \mathbf{p}}^{(4)} U_{\sigma s}(\theta) \\ &\quad \times d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) D_{\mathbf{p}, \lambda}(t) - \text{H.c.}], \end{aligned} \quad (29)$$

$$\begin{aligned} I_5(t) &= -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, \nu, s} \sum_i \sum_{\mathbf{p}, \lambda} \sqrt{\omega_{\mathbf{p}, \lambda}} [T_{i, \mathbf{k}, \mathbf{q}, \mathbf{p}}^{(5)} \mathbf{S}_i \cdot \vec{\tau}_{\sigma \nu} \\ &\quad \times U_{\nu s}(\theta) d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) D_{\mathbf{p}, \lambda}(t) - \text{H.c.}], \end{aligned} \quad (30)$$

$$\begin{aligned} I_6(t) &= -i \sum_{\mathbf{k}, \mathbf{q}} \sum_{\sigma, s} \sum_{i \neq j} \sum_{\mathbf{p}, \lambda} \sqrt{\omega_{\mathbf{p}, \lambda}} [T_{i, j, \mathbf{k}, \mathbf{q}, \mathbf{p}}^{(6)} U_{\sigma s}(\theta) \\ &\quad \times d_{\mathbf{k}, \sigma}^\dagger(t) f_{\mathbf{q}, s}(t) D_{\mathbf{p}, \lambda}(t) - \text{H.c.}], \end{aligned} \quad (31)$$

where $I_1(t), \dots, I_6(t)$ arise from the contributions of H_1, \dots, H_6 , respectively. With Eq. (24) and Eq. (25), the Green's function $\langle \langle I(t) | H'(t') \rangle \rangle$ can be represented by the following four GFs:

$$\begin{aligned} \langle \langle I(t) | H'(t') \rangle \rangle &= \langle \langle I_1(t) + I_3(t) | H_1(t') + H_3(t') \rangle \rangle \\ &\quad + \langle \langle I_2(t) | H_2(t') \rangle \rangle + \langle \langle I_4(t) + I_6(t) | H_4(t') \\ &\quad + H_6(t') \rangle \rangle + \langle \langle I_5(t) | H_5(t') \rangle \rangle, \end{aligned} \quad (32)$$

the other GFs, such as $\langle \langle I_1(t) | H_2(t') \rangle \rangle$, being all of zero. Equations (11)–(16) and (26)–(31) indicate that the four Green's functions on the right-hand side of Eq. (32) describe the non-spin-flip, spin-flip, phonon-assisted non-spin-flip, and phonon-assisted spin-flip tunneling processes, respectively. The non-spin-flip GF $\langle \langle I_1(t) + I_3(t) | H_1(t') + H_3(t') \rangle \rangle$ can be obtained as in the Refs. 15,16, and the phonon-assisted non-spin-flip GF $\langle \langle I_4(t) + I_6(t) | H_4(t') + H_6(t') \rangle \rangle$ as in the Ref. 16. As for the two spin-flip GFs $\langle \langle I_2(t) | H_2(t') \rangle \rangle$ and $\langle \langle I_5(t) | H_5(t') \rangle \rangle$, the factorization $\langle S_i^x S_j^y \rangle = \delta_{i,j} \delta_{x,y} \langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle / 3 = \delta_{i,j} \delta_{x,y} / 4$ ($S = 1/2$) is adopted where the correlation between different sites has been neglected, and the polarization effect of the barrier by the magnetic electrodes has also been omitted because the Mössbauer spectroscopy indicates that the barrier is nonmagnetic.¹¹ After this factorization, $\langle \langle I_2(t) | H_2(t') \rangle \rangle$ and $\langle \langle I_5(t) | H_5(t') \rangle \rangle$ can be obtained by the procedures as for $\langle \langle I_1(t) + I_3(t) | H_1(t') + H_3(t') \rangle \rangle$ and $\langle \langle I_4(t) + I_6(t) | H_4(t') + H_6(t') \rangle \rangle$, respectively. Substituting the four GFs into Eq. (32) and then into Eq. (22), we arrive finally at

$$\begin{aligned}
I = & \pi e \sum_{\mathbf{k}, \mathbf{q}} \left| T_{\mathbf{k}, \mathbf{q}}^{(1)} + \sum_{i, j} T_{i, j, \mathbf{k}, \mathbf{q}}^{(3)} \right|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \left[\sum_{\sigma, \sigma'} \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) + \cos(\theta) \sum_{\sigma, \sigma'} \sigma \sigma' \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) \right] \\
& \times [f(\omega_1) - f(\omega_2)] \delta(\omega_2 - \omega_1 - eV) + \pi e \sum_{\mathbf{k}, \mathbf{q}} \sum_i |T_{i, \mathbf{k}, \mathbf{q}}^{(2)}|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \left[\frac{3}{4} \sum_{\sigma, \sigma'} \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) \right. \\
& \left. - \frac{1}{4} \cos(\theta) \sum_{\sigma, \sigma'} \sigma \sigma' \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) \right] [f(\omega_1) - f(\omega_2)] \delta(\omega_2 - \omega_1 - eV) + \pi e \sum_{\mathbf{k}, \mathbf{q}} \sum_{\mathbf{p}, \lambda} \omega_{\mathbf{p}, \lambda} \left| T_{\mathbf{k}, \mathbf{q}, \mathbf{p}}^{(4)} \right. \\
& \left. + \sum_{i, j} T_{i, j, \mathbf{k}, \mathbf{q}, \mathbf{p}}^{(6)} \right|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_3}{2\pi} \\
& \times \mathcal{A}_D^{(\lambda)}(\mathbf{p}, \omega_3) \left[\sum_{\sigma, \sigma'} \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) + \cos(\theta) \sum_{\sigma, \sigma'} \sigma \sigma' \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) \right] [f(\omega_2 + \omega_3) - f(\omega_1)] \\
& \times [b(\omega_3) - f(\omega_2)] \delta(\omega_2 + \omega_3 - \omega_1 + eV) + \pi e \sum_{\mathbf{k}, \mathbf{q}} \sum_{\mathbf{p}, \lambda} \omega_{\mathbf{p}, \lambda} \sum_i |T_{i, \mathbf{k}, \mathbf{q}, \mathbf{p}}^{(5)}|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_3}{2\pi} \\
& \times \mathcal{A}_D^{(\lambda)}(\mathbf{p}, \omega_3) \left[\frac{3}{4} \sum_{\sigma, \sigma'} \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) - \frac{1}{4} \cos(\theta) \sum_{\sigma, \sigma'} \sigma \sigma' \Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) \right] [f(\omega_2 + \omega_3) - f(\omega_1)] \\
& \times [b(\omega_3) - f(\omega_2)] \delta(\omega_2 + \omega_3 - \omega_1 + eV), \tag{33}
\end{aligned}$$

where V is the bias voltage, $f(\omega)$ and $b(\omega)$ denote the Fermi and Bose distribution functions respectively, and

$$\mathcal{A}_D^{(\lambda)}(\mathbf{p}, \omega) = -2 \text{Im} \langle \langle D_{\mathbf{p}, \lambda} | D_{\mathbf{p}, \lambda}^\dagger \rangle \rangle_{\omega + i0^+}, \tag{34}$$

$$\Phi_{\sigma, \sigma'}(\mathbf{k}, \omega_1; \mathbf{q}, \omega_2) = \mathcal{A}_d^{(\sigma)}(\mathbf{k}, \omega_1) \mathcal{A}_f^{(\sigma')}(\mathbf{q}, \omega_2), \tag{35}$$

with

$$\mathcal{A}_d^{(\sigma)}(\mathbf{k}, \omega) = -2 \text{Im} \langle \langle d_{\mathbf{k}, \sigma} | d_{\mathbf{k}, \sigma}^\dagger \rangle \rangle_{\omega + i0^+}, \tag{36}$$

$$\mathcal{A}_f^{(\sigma)}(\mathbf{q}, \omega) = -2 \text{Im} \langle \langle f_{\mathbf{q}, \sigma} | f_{\mathbf{q}, \sigma}^\dagger \rangle \rangle_{\omega + i0^+}, \tag{37}$$

where $\langle \langle A|B \rangle \rangle_z$ represents the retarded Green's function of A and B on the complex z plane,

$$\langle \langle d_{\mathbf{k}, \sigma} | d_{\mathbf{k}, \sigma}^\dagger \rangle \rangle_z = \frac{1}{z - \epsilon_{\mathbf{k}, \sigma}}, \tag{38}$$

$$\langle \langle f_{\mathbf{q}, \sigma} | f_{\mathbf{q}, \sigma}^\dagger \rangle \rangle_z = \frac{1}{z - \zeta_{\mathbf{q}, \sigma}}, \tag{39}$$

$$\langle \langle D_{\mathbf{p}, \lambda} | D_{\mathbf{p}, \lambda}^\dagger \rangle \rangle_z = \frac{1}{z - \omega_{\mathbf{p}, \lambda}} + \frac{1}{z + \omega_{\mathbf{p}, \lambda}}, \tag{40}$$

which are obtained from the H_0 of Eq. (9).

If there exists only the direct tunneling, i.e., $H' = H_1$, and the electrodes are non-magnetic, Eq. (33) reduces to the well-known result of the direct tunneling current between two normal metals,^{15,16}

$$\begin{aligned}
I = & 4\pi e \sum_{\mathbf{k}, \mathbf{q}} |T_{\mathbf{k}, \mathbf{q}}^{(1)}|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \mathcal{A}_d(\mathbf{k}, \omega_1) \mathcal{A}_f(\mathbf{q}, \omega_2) \\
& \times [f(\omega_1) - f(\omega_2)] \delta(\omega_2 - \omega_1 - eV), \tag{41}
\end{aligned}$$

where $\mathcal{A}_d(\mathbf{k}, \omega) = \mathcal{A}_d^{(\sigma)}(\mathbf{k}, \omega) = \mathcal{A}_d^{(-\sigma)}(\mathbf{k}, \omega)$, and $\mathcal{A}_f(\mathbf{q}, \omega) = \mathcal{A}_f^{(\sigma)}(\mathbf{q}, \omega) = \mathcal{A}_f^{(-\sigma)}(\mathbf{q}, \omega)$. If $H' = H_4$, and the electrodes are nonmagnetic, Eq. (33) reduces to the usual result for phonon-assisted tunneling current:¹⁶

$$\begin{aligned}
I = & 4\pi e \sum_{\mathbf{k}, \mathbf{q}} \sum_{\mathbf{p}, \lambda} \omega_{\mathbf{p}, \lambda} |T_{\mathbf{k}, \mathbf{q}, \mathbf{p}}^{(4)}|^2 \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega_2}{2\pi} \\
& \times \int_{-\infty}^{+\infty} \frac{d\omega_3}{2\pi} \mathcal{A}_D^{(\lambda)}(\mathbf{p}, \omega_3) \mathcal{A}_d(\mathbf{k}, \omega_1) \mathcal{A}_f(\mathbf{q}, \omega_2) \\
& \times [f(\omega_2 + \omega_3) - f(\omega_1)] [b(\omega_3) - f(\omega_2)] \\
& \times \delta(\omega_2 + \omega_3 - \omega_1 + eV). \tag{42}
\end{aligned}$$

The combined influence of H_1, \dots, H_6 makes the tunneling current somewhat complicated since it includes now four terms, as indicated in Eq. (33). Physically, they represent the contributions from the non-spin-flip, spin-flip, phonon-assisted non-spin-flip, and phonon-assisted spin-flip tunneling processes, respectively. For simplicity, we assume hereafter that the two ferromagnetic electrodes are made of the same material.

According to Ref. 12, the six tunneling matrices can be approximated as

$$A(t) = T_{\mathbf{k}, \mathbf{q}}^{(1)} = A_0 e^{-\kappa t}, \tag{43}$$

$$|B(t)|^2 = \sum_i |T_{i,\mathbf{k},\mathbf{q}}^{(2)}|^2 = B_0^2 e^{-(\alpha+\kappa)t}, \quad (44)$$

$$C(t) = \sum_{i,j} T_{i,j,\mathbf{k},\mathbf{q}}^{(3)} = C_0 e^{-\alpha t}, \quad (45)$$

$$A'(t) = T_{\mathbf{k},\mathbf{q},\mathbf{p}}^{(4)} = A_1 e^{-\kappa t}, \quad (46)$$

$$|B'(t)|^2 = \sum_i |T_{i,\mathbf{k},\mathbf{q},\mathbf{p}}^{(5)}|^2 = B_1^2 e^{-(\alpha+\kappa)t}, \quad (47)$$

$$C'(t) = \sum_{i,j} T_{i,j,\mathbf{k},\mathbf{q},\mathbf{p}}^{(6)} = C_1 e^{-\alpha t}, \quad (48)$$

where A_0 , B_0 , C_0 , A_1 , B_1 , and C_1 are constants, and the κ and α stand for the decay factor of the wave function $\phi_{l\mathbf{k}}(\mathbf{r})$ in the barrier region and the localization coefficient of the localized state $w(\mathbf{r}-\mathbf{R}_i)$, respectively. Here, as a preliminary approximation, the Bloch wave function $\phi_{l\mathbf{k}}(\mathbf{r})$ is treated within the free-electron model, which results in a single-decay rate κ . To improve this approximation, one should take into account the influence of the lateral symmetry¹⁸ on $\phi_{l\mathbf{k}}(\mathbf{r})$ by the layer KKR (Korringa-Kohn-Rostoker) approach, which is a generalization to the free-electron model for the calculating of the tunneling conductance, and can be applied to real materials.¹⁹

By using the approximations of Eqs. (43)–(48), Eq. (33) can be simplified as follows:

$$\begin{aligned} I = & \pi e \left[\left(|A(t) + C(t)|^2 + \frac{3}{4} |B(t)|^2 \right) \sum_{\sigma,\sigma'} g_{\sigma}(0) g_{\sigma'}(0) \right. \\ & + \cos(\theta) \left(|A(t) + C(t)|^2 - \frac{1}{4} |B(t)|^2 \right) \sum_{\sigma,\sigma'} \sigma \sigma' g_{\sigma}(0) \\ & \times g_{\sigma'}(0) \left. \int_{-\infty}^{+\infty} d\omega_2 [f(\omega_2 - eV) - f(\omega_2)] + \pi e \left[\left(|A'(t) \right. \right. \right. \\ & + C'(t)|^2 + \frac{3}{4} |B'(t)|^2 \left. \left. \right) \sum_{\sigma,\sigma'} g_{\sigma}(0) g_{\sigma'}(0) + \cos(\theta) \right. \\ & \times \left. \left(|A'(t) + C'(t)|^2 - \frac{1}{4} |B'(t)|^2 \right) \sum_{\sigma,\sigma'} \sigma \sigma' g_{\sigma}(0) g_{\sigma'}(0) \right] \\ & \times \sum_{\mathbf{p},\lambda} \omega_{\mathbf{p},\lambda} \int_{-\infty}^{+\infty} d\omega_2 \{ [f(\omega_2 + \omega_{\mathbf{p},\lambda}) - f(\omega_2 + \omega_{\mathbf{p},\lambda} + eV)] \\ & \times [b(\omega_{\mathbf{p},\lambda}) - f(\omega_2)] - [f(\omega_2 - \omega_{\mathbf{p},\lambda}) \\ & - f(\omega_2 - \omega_{\mathbf{p},\lambda} + eV)] [b(-\omega_{\mathbf{p},\lambda}) - f(\omega_2)] \}, \quad (49) \end{aligned}$$

where, as usual, we have taken the approximation: $\sum_{\mathbf{k}} \mathcal{A}_d^{(\sigma)}(\mathbf{k}, \omega) / 2\pi = g_{\sigma}(0)$ with $g_{\sigma}(0)$ being the density of states (DOS) of the electrons with spin σ at the Fermi level. Considering the fact that the measured temperature in the

experiments^{4–11} is far lower than the Fermi temperature of the electron gases in the two electrodes, $f(\omega) \approx \vartheta(-\omega)$, where $\vartheta(\omega)$ denotes the step function. Thus, we obtain

$$\begin{aligned} I = & \pi e \left[\left(|A(t) + C(t)|^2 + \frac{3}{4} |B(t)|^2 \right) \sum_{\sigma,\sigma'} g_{\sigma}(0) g_{\sigma'}(0) \right. \\ & + \cos(\theta) \left(|A(t) + C(t)|^2 - \frac{1}{4} |B(t)|^2 \right) \sum_{\sigma,\sigma'} \sigma \sigma' g_{\sigma}(0) \\ & \times g_{\sigma'}(0) \left. \right] \cdot eV + \pi e \left[\left(|A'(t) + C'(t)|^2 + \frac{3}{4} |B'(t)|^2 \right) \right. \\ & \times \sum_{\sigma,\sigma'} g_{\sigma}(0) g_{\sigma'}(0) + \cos(\theta) \left(|A'(t) + C'(t)|^2 \right. \\ & \left. - \frac{1}{4} |B'(t)|^2 \right) \sum_{\sigma,\sigma'} \sigma \sigma' g_{\sigma}(0) g_{\sigma'}(0) \left. \right] \\ & \times \sum_{\mathbf{p},\lambda} \omega_{\mathbf{p},\lambda} [2eV b(\omega_{\mathbf{p},\lambda}) + (eV - \omega_{\mathbf{p},\lambda}) \vartheta(eV - \omega_{\mathbf{p},\lambda})]. \quad (50) \end{aligned}$$

The derivative of I with respect to V gives the tunneling conductance G ,

$$\begin{aligned} G(\theta) = & \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \left\{ \left(|A(t) + C(t)|^2 + \frac{3}{4} |B(t)|^2 \right) \right. \\ & + \cos(\theta) \left(|A(t) + C(t)|^2 - \frac{1}{4} |B(t)|^2 \right) P^2 \left. \right\} \\ & + \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \\ & \times \left\{ \left(|A'(t) + C'(t)|^2 + \frac{3}{4} |B'(t)|^2 \right) \right. \\ & + \cos(\theta) \left(|A'(t) + C'(t)|^2 - \frac{1}{4} |B'(t)|^2 \right) P^2 \left. \right\} \\ & \times \sum_{\mathbf{p},\lambda} \omega_{\mathbf{p},\lambda} [2b(\omega_{\mathbf{p},\lambda}) + \vartheta(eV - \omega_{\mathbf{p},\lambda})], \quad (51) \end{aligned}$$

where

$$P = \frac{g_{\uparrow}(0) - g_{\downarrow}(0)}{g_{\uparrow}(0) + g_{\downarrow}(0)} \quad (52)$$

represents the spin polarization of the DOS in the ferromagnet. Usually, the bias voltage V is very small when compared with the Debye frequency ω_D , i.e., $eV \ll \hbar \omega_D$, this means that the tunneling conductance can be approximated as

$$\begin{aligned}
G(\theta) = & \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \left\{ \left(|A(t) + C(t)|^2 + \frac{3}{4} |B(t)|^2 \right) \right. \\
& + \cos(\theta) \left(|A(t) + C(t)|^2 - \frac{1}{4} |B(t)|^2 \right) P^2 \left. \right\} \\
& + 8 \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \left(\frac{T}{\Theta} \right)^4 \\
& \times D \left(\frac{\Theta}{T} \right) \left\{ \left(|\tilde{A}'(t) + \tilde{C}'(t)|^2 + \frac{3}{4} |\tilde{B}'(t)|^2 \right) \right. \\
& + \cos(\theta) \left(|\tilde{A}'(t) + \tilde{C}'(t)|^2 - \frac{1}{4} |\tilde{B}'(t)|^2 \right) P^2 \left. \right\}, \quad (53)
\end{aligned}$$

where $\Theta = \omega_D/k_B$ is the Debye temperature,

$$D\left(\frac{\Theta}{T}\right) = \int_0^{\Theta/T} dx \frac{x^3}{e^x - 1} \quad (54)$$

the Debye function, and

$$\tilde{A}'(t) = \sqrt{9N\omega_D/8} A'(t) = \tilde{A}_1 e^{-\kappa t}, \quad (55)$$

$$\tilde{B}'(t) = \sqrt{9N\omega_D/8} B'(t) = \tilde{B}_1 e^{-(\alpha+\kappa)t/2}, \quad (56)$$

$$\tilde{C}'(t) = \sqrt{9N\omega_D/8} C'(t) = \tilde{C}_1 e^{-\alpha t}. \quad (57)$$

If only the direct tunneling term H_1 is considered in H' , Eq. (53) reduces simply to Jullière's result:

$$J = \frac{2P^2}{1+P^2}. \quad (58)$$

If we consider further the contributions from the terms of H_2, \dots, H_6 , i.e., if the effects of the phonons and localized states in the amorphous barrier on the tunneling processes are incorporated, the magnetoconductance is seriously modified, as indicated in Eq. (53). As will be shown below, this modification will lead to two new features of the magnetoconductance-difference: the oscillation with the increasing barrier thickness and the enhancement with the elevating temperature.

According to the definition of Eq. (3), we can obtain the magnetoconductance-difference ΔG from Eq. (53) as follows:

$$\begin{aligned}
\Delta G = & G_P - G_A = G(0) - G(\pi) \\
= & 2 \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \left\{ \left(|A(t) + C(t)|^2 \right. \right. \\
& - \frac{1}{4} |B(t)|^2 \left. \right) + 8 \left(\frac{T}{\Theta} \right)^4 D \left(\frac{\Theta}{T} \right) \left(|\tilde{A}'(t) + \tilde{C}'(t)|^2 \right. \\
& \left. \left. - \frac{1}{4} |\tilde{B}'(t)|^2 \right) \right\} P^2. \quad (59)
\end{aligned}$$

It describes the varying rate of the tunneling conductance as the magnetizations of the two electrodes change from mutual

parallel to mutual antiparallel under the drive of an external magnetic field. As shown by Eqs. (1) and (2), it is directly proportional to the JMR or TMR, namely, the larger the ΔG , the higher the JMR or TMR. In a word, it reflects physically the intrinsic properties of the JMR or TMR of a magnetic tunnel junction.

At zero temperature, Eq. (59) becomes

$$\begin{aligned}
\Delta G = & 2 \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \\
& \times \left(|A(t) + C(t)|^2 - \frac{1}{4} |B(t)|^2 \right) P^2. \quad (60)
\end{aligned}$$

Just as the interlayer exchange coupling for the zero temperature,¹² there are two competing contributions to the magnetoconductance-difference: the term proportional to $|A(t) + C(t)|^2$ and the term proportional to $|B(t)|^2$. Physically, the former comes from the non-spin-flip tunneling produced by the Hamiltonians H_1 and H_3 , and it yields a positive contribution; the latter comes from the spin-flip tunneling produced by the Hamiltonians H_2 , and it yields a negative contribution. The net value of the magnetoconductance-difference is determined by the competition between the non-spin-flip tunneling and spin-flip tunneling: in the region where the non-spin-flip tunneling dominates, i.e., $|A(t) + C(t)|^2 > |B(t)|^2/4$, the net value of ΔG is positive; in the region where the spin-flip tunneling dominates, i.e., $|A(t) + C(t)|^2 < |B(t)|^2/4$, the net value of ΔG is negative. As pointed out in Ref. 12, $\alpha > \kappa$ for a -Si and a -Ge, Eqs. (43)–(45) show that $C(t)$ attenuates more quickly than $B(t)$, and $B(t)$ attenuates more quickly than $A(t)$, as a result, if $B(t)$ is large enough, there will appear a negative region in the middle range of the barrier thickness, with the positive regions occupying the two sides of it. In other words, the magnetoconductance-difference will oscillate

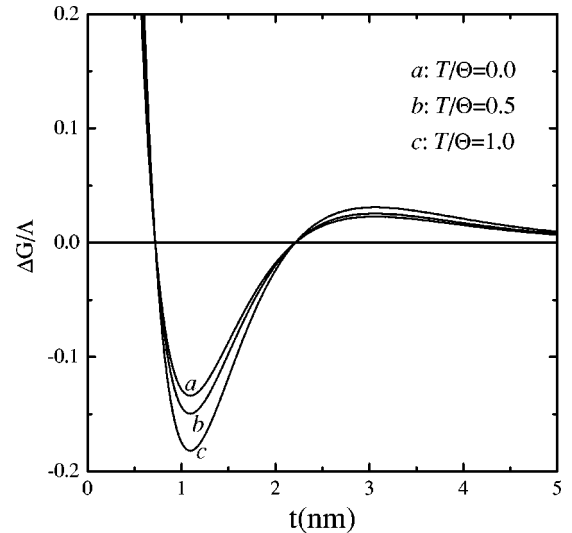


FIG. 1. The magnetoconductance-difference vs the barrier thickness for different temperatures. Here, $\Lambda = 2 \pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 A_0^2 P^2$, $\kappa^{-1} = 2$ nm, $\alpha^{-1} = 0.8$ nm, $B_0/A_0 = 7.2$, $C_0/A_0 = 3.0$, $\tilde{A}_1/A_0 = 0.5$, $\tilde{B}_1/A_0 = 3.6$, and $\tilde{C}_1/A_0 = 1.5$, and $T/\Theta = 0.0, 0.5$, and 1.0 for curves a, b , and c , respectively.

from positive to negative and back to positive values with the increase of the barrier thickness at zero temperature if the spin-flip tunneling is strong enough. For the exchange coupling, this competition causes it to oscillate with the barrier thickness too.¹² Therefore, the mechanism responsible for the oscillation of the exchange coupling is also responsible for the oscillation of the magnetoconductance-difference.

At finite temperatures, Eq. (59) indicates that there arises a new contribution to the magnetoconductance-difference:

$$16\pi e^2 [g_{\uparrow}(0) + g_{\downarrow}(0)]^2 \cdot \left(\frac{T}{\Theta}\right)^4 \times D\left(\frac{\Theta}{T}\right) \cdot \left(|\tilde{A}'(t) + \tilde{C}'(t)|^2 - \frac{1}{4} |\tilde{B}'(t)|^2 \right) P^2. \quad (61)$$

It originates from the phonon-assisted tunneling produced by the Hamiltonians H_4 , H_5 , and H_6 , and gives no contribution at zero temperature. For the same reason as above, this term will oscillate with the variation of the barrier thickness as well, which can be seen directly by comparing Eqs. (43)–(45) with Eqs. (46)–(48) or Eqs. (55)–(57). More importantly, this term will enlarge the magnitude of the magnetoconductance-difference with the increasing of temperature because, as well-known, the factor $(T/\Theta)^4 D(T/\Theta)$

increases monotonically with the temperature T . That is to say, the magnetoconductance-difference is heat activated at finite temperatures. Reference 13 demonstrates that this phonon-assisted tunneling also accounts for the heat-activation behavior of the interlayer exchange coupling at finite temperatures, which means that the mechanism for the heat activation of the magnetoconductance-difference is the same as that for the interlayer exchange coupling. These two features of the oscillation and heat-activation of the magnetoconductance-difference are shown clearly in Fig. 1.

In conclusion, by taking into account the effects of the indirect tunnelings through the phonons and the localized states in the amorphous barrier, we have demonstrated that the magnetoconductance-difference for the tunnel junction with an amorphous-semiconducting barrier can oscillate with the variation of the barrier thickness, and can increase with the elevation of temperature. The mechanism for these features is just the same as that for the oscillation and heat activation of the interlayer exchange coupling suggested in our previous works,^{12,13} which have explained the experimental data successfully. Thus, we believe that the oscillation and heat activation of the magnetoconductance-difference could also be observed in future experiments.

This work was supported by the State Key Project of Fundamental Research under Grant No. 001CB610602.

¹M. Jullière, Phys. Lett. **54A**, 225 (1975).

²S. Maekawa and D. Gáfvert, IEEE Trans. Magn. **18**, 707 (1982).

³R. Meservey and P. M. Tedrow, Phys. Rep. **238**, 173 (1994).

⁴S. Toscano, B. Briner, H. Hipster, and M. Landolt, J. Magn. Magn. Mater. **114**, L6 (1992).

⁵E. E. Füllerton, J. E. Mattson, S. R. Lee, C. H. Sowers, Y. Y. Huang, G. Felcher, and S. D. Bader, J. Magn. Magn. Mater. **117**, L301 (1992).

⁶E. E. Füllerton, J. E. Mattson, S. R. Lee, C. H. Sowers, Y. Y. Huang, G. Felcher, and S. D. Bader, J. Appl. Phys. **73**, 6335 (1993).

⁷C. L. Foiles, M. R. Franklin, and R. Loloee, Phys. Rev. B **50**, 16070 (1994).

⁸B. Briner and M. Landolt, Z. Phys. B: Condens. Matter **92**, 137 (1993).

⁹B. Briner, U. Ramsperger, and M. Landolt, Phys. Rev. B **51**, 7303 (1995).

¹⁰B. Briner and M. Landolt, Phys. Rev. Lett. **73**, 340 (1994).

¹¹J. E. Mattson, S. Kumar, E. E. Füllerton, S. R. Lee, C. H. Sowers, M. Grimsditch, S. D. Bader, and F. T. Parker, Phys. Rev. Lett. **71**, 185 (1993).

¹²M. W. Xiao and Z. Z. Li, Phys. Rev. B **54**, 3322 (1996).

¹³M. W. Xiao, Z. Z. Li, and W. Xu, Chin. Phys. Lett. **19**, 1691 (2002).

¹⁴J. S. Moodera and G. Mathon, J. Magn. Magn. Mater. **200**, 248 (1999).

¹⁵G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).

¹⁶C. B. Duke, *Tunneling in Solids* (Academic, New York, 1969).

¹⁷D. N. Zubrev, *Nonequilibrium Statistical Thermodynamics* (Consultants Bureau, New York, 1974).

¹⁸W. H. Butler, X. -G. Zhang, T. C. Schulthess, and J. M. MacLaren, Phys. Rev. B **63**, 092402 (2001).

¹⁹J. M. MacLaren, X. -G. Zhang, W. H. Butler, and Xindong Wang, Phys. Rev. B **59**, 5470 (1999).