

Magnetic diode effect in double-barrier tunnel junctions

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Abstract. – A quantum-statistical theory of spin-dependent tunneling through asymmetric magnetic double-barrier junctions is presented which describes *both* ballistic and diffuse tunneling by a single analytical expression. It is evidenced that the key parameter for the transition between these two tunneling regimes is the electron scattering. For these junctions a strong asymmetric behaviour in the I - V characteristics and the tunnel magnetoresistance (TMR) is predicted which can be controlled by an applied magnetic field. This phenomenon relates to the quantum well states in the middle metallic layer. The corresponding resonances in the current and the TMR are drastically phase-shifted under positive and negative voltage.

After the discovery of a large room temperature magnetoresistance effect in magnetic tunnel junctions (MTJ) [1] many potential applications have emerged based on the spin-polarized transport through a thin insulating barrier sandwiched between two ferromagnetic metals [1–4]. The current state-of-the-art production of tunnel junction elements with a resistance variation of up to 40% when magnetically switched [5,6] makes them very promising in particular for the application as tunneling magnetic random access memories (MRAM). Current MRAM designs [5, 7] which incorporate arrays of magnetic tunnel junctions add an additional semiconductor switch in series (either a CMOS transistor or a p - n junction) with the MTJ memory cell to suppress (or block) parasitic signal paths within the array of lines. However, such a concept is hampered by the difficulty of mixing semiconductor and metal technology. In this letter, we propose a novel theoretical concept which eliminates the introduction of additional semiconductor components by using an asymmetric double-barrier structure M_1/O_2 a/M_3 b/O_4 c/M_5 (M_i and O_i are the magnetic metal and oxide layer, respectively with corresponding thickness a , b and c) that in itself acts as the blocking device. It is shown that the I - V characteristics and the TMR of such asymmetric double-barrier structures have a strong “diode”-like behaviour under positive and negative applied voltage. Moreover, the asymmetric properties can be varied by a magnetic field leading to the concept of a “magnetically controlled” diode.

The potential profile of the system under applied voltage V_{ext} is shown in fig. 1(a), where U_i and V_i ($i = 2, 4$) are, respectively, the potential of the barrier region and the linear voltage drop therein, and V_i^σ ($i = 1, 3, 5$) is the spin-dependent potential of the i -th metal. The outer

metallic layers are assumed to be semi-infinite. The symmetric structures with $a = c$ and $U_2 = U_4$ were considered in refs. [8,9] but the resonance tunneling was described without taking into account the electron's scattering inside the middle metallic layer. In this case it was shown that the conductivity and the TMR exhibit resonance peaks as a function of the thickness of the middle metallic layer due to quantum well states. Here we will show that the asymmetry of the structure in combination with the presence of quantum well states leads to a large asymmetry in the current for forward (positive) and reverse (negative) applied voltage. The evaluation of the current through the double-barrier junction is based on the determination of its transmission probability D [10]. Here, D is derived using the Green functions technique in the mixed real space-momentum representation [11–13] and it can be written in the form

$$D = \left(\frac{\hbar^2}{2m} \right)^2 \left\{ \left[\frac{\partial G_\kappa}{\partial z} - \frac{\partial G_\kappa^*}{\partial z} \right] \left[\frac{\partial G_\kappa}{\partial z'} - \frac{\partial G_\kappa^*}{\partial z'} \right] - \left[\frac{\partial^2 G_\kappa}{\partial z \partial z'} - \frac{\partial^2 G_\kappa^*}{\partial z \partial z'} \right] [G_\kappa - G_\kappa^*] \right\}, \quad (1)$$

where $G_\kappa \equiv G_\kappa(z, z')$ and $G_\kappa^* \equiv G_\kappa^*(z, z')$ are retarded and advanced Green functions of the system, z is the coordinate perpendicular to the plane of the structure and κ indicates the in-plane momentum of the electron. This expression is similar to the Kubo formula for the non-local conductivity [12] by replacing Fermi energy E_F with an arbitrary energy E over which an integration has to be done in the limits from E_F up to $E_F + eV_{\text{ext}}$. It is convenient to use eq. (1) since, for the calculation of the Green function of a system including scattering, it is possible to use well-defined quantum-statistical methods. In the presence of scattering in the metallic layers, the problem cannot be solved exactly and the tunneling through the whole system is described by consecutive tunneling through each barrier. In this case the current densities in the first and second barrier are calculated separately and the condition of constant current throughout the structure has to be fulfilled by introducing either an effective electrical field [13,14] inside each barrier or by calculating the so-called vertex correction [13,15]. Here the first approach is used. The Green function is the solution to the Schrödinger equation in each layer, where in the barrier region the WKB approximation [16] is used:

$$\left(E + \frac{\hbar^2}{2m_i} \left(\frac{\partial^2}{\partial z^2} - \kappa^2 \right) - V_i^\sigma + i \frac{\hbar^2 k_{Ei}^\sigma}{m_i l_i^\sigma} - eV_i(z) \right) G_\kappa(z, z') = \delta(z - z'), \quad (i = 1, 3, 5)$$

and

$$\left(E + \frac{\hbar^2}{2m_i} \left(\frac{\partial^2}{\partial z^2} - \kappa^2 \right) - (U_i + eV_i(z)) \right) G_\kappa(z, z') = \delta(z - z'), \quad (i = 2, 4),$$

where $k_{Ei}^\sigma = \sqrt{(2m_i/\hbar^2)(E - V_i^\sigma)}$, l_i^σ and m_i are the mean free path of the electron with energy E and spin σ and its effective mass in the i -th layer, respectively, and voltage

$$V_i(z) = \begin{cases} 0, & z < 0, \\ (zV_2)/a, & 0 < z < a, \\ V_2, & a < z < a + b, \\ V_2 + (z - a - b)V_4/c, & a + b < z < a + b + c, \\ V_{\text{ext}}, & z > a + b + c. \end{cases}$$

The solutions in each layer are matched by the boundary condition at the interfaces $z = 0$, a , $a + b$, $a + b + c$ (see fig. 1(a)). From the Green function the non-local probability D is

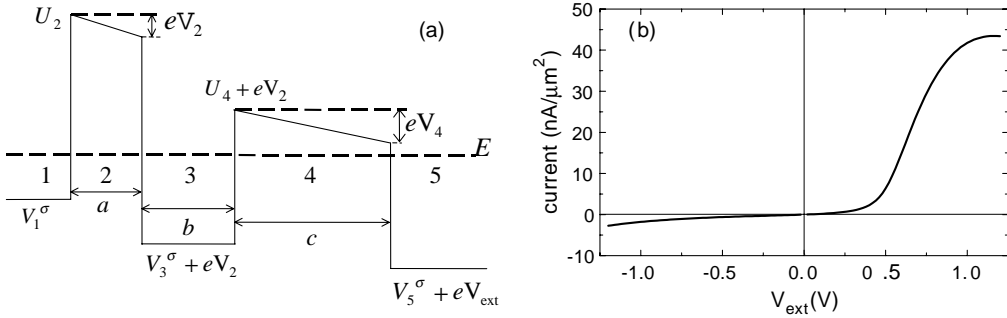


Fig. 1 – (a) Potential energy diagram and (b) the calculated current-voltage curve for the asymmetric structure Cu/O₂ 7 Å/Cu 5.5 Å/O₄ 21 Å/Cu, with $U_2 - E_F = U_4 - E_F = 3$ eV.

calculated using the formula (1). With the assumption that the voltage drop occurs only across the barrier regions (V_2 and V_4 in fig. 1(a)) and that the conduction band edge is flat in the metallic regions, it is sufficient to consider only the non-local probability for those z and z' lying in the barrier regions 2, 4 [11] (see fig. 1(a)). This yields the four analytical expressions: D_{22} , D_{24} , D_{42} and D_{44} . It is found that these quantities are independent of z and z' and hence the condition that the divergence of the current density is zero is automatically satisfied inside the different regions. With these two-point tunneling probabilities the current density throughout the first (j_2) and the second (j_4) barrier can be calculated separately and are written in the following form, ref. [10]:

$$j_{2(4)}^\sigma = \frac{e}{\pi h} \int dE [f(E) - f(E + eV_2)] \int D_{22(42)}^\sigma(E, \kappa) \kappa d\kappa + \frac{e}{\pi h} \int dE [f(E + eV_2) - f(E + eV_{\text{ext}})] \int D_{24(44)}^\sigma(E, \kappa) \kappa d\kappa, \quad (2)$$

where $f(E)$ is the thermal occupation probability of a state with energy E . This is the generalization of the linear response in metals where the current density at a point z is related to the electric field at a point z' through the two-point conductivity $\sigma(z, z')$. Finally, from

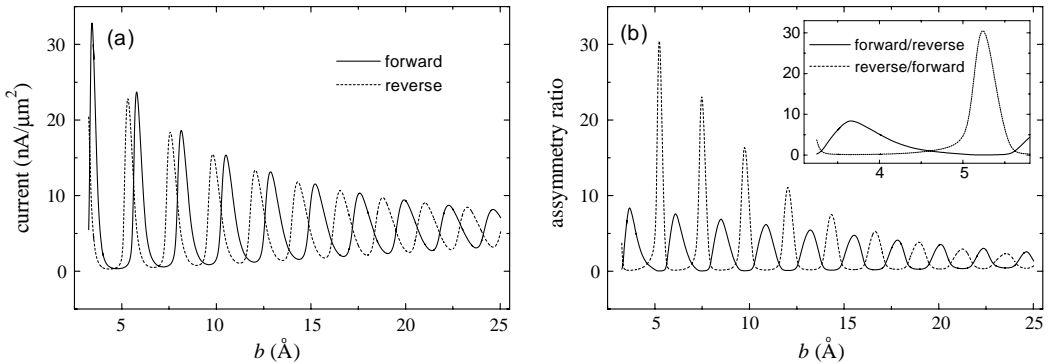


Fig. 2 – Dependence of (a) the forward and reverse current and (b) the corresponding asymmetry ratio on the layer thickness b of the middle metallic layer for the non-magnetic asymmetric double-barrier structure (see text).

the requirement that the current density has to be constant throughout the whole barrier structure, $j_2^g = j_4^g$, the effective electric field inside each barrier and hence the voltage drops V_2 and V_4 are determined in a self-consistent way for a given applied voltage V_{ext} . The additional condition of the current conservation here results from introducing the effective electric field instead of calculating the vertex corrections [14]. Alternatively, if one calculates the current taking into account the vertex correction, the matching of the boundary conditions would be enough to provide the current conservation. The resulting dependence of the current density on V_{ext} is given in fig. 1(b) for the case of an asymmetric double-barrier structure $a \neq c$ or $U_2 \neq U_4$, revealing a strong asymmetry in the I - V characteristic reminiscent of a diode. To understand the physical origin of this enhanced asymmetry, we first consider the case where M_1 , M_3 and M_5 are non-magnetic metals, using for the Fermi wave vector the value of Cu $k_{E_F i} = 1.36 \text{ \AA}^{-1}$ [17]. Cu is chosen here because of its simple electronic structure similar to free electrons. Furthermore, we use the electron mean free path of 100 \AA for the scattering in the metallic layers and an electron effective mass of $m_{2(4)} = 0.4$ [18] inside the barriers. In fig. 2(a) the current density is shown as a function of the thickness b of the middle layer M_3 for a fixed applied voltage $V_{\text{ext}} = 0.7 \text{ V}$ for a double-barrier structure of Cu/ O_2 21 \AA /Cu $b \text{ \AA}$ / O_4 21 \AA /Cu with different barrier heights ($U_2 - E_F = 1 \text{ eV}$ and $U_4 - E_F = 3 \text{ eV}$). Both forward (positive V_{ext}) and reverse (negative V_{ext}) currents exhibit resonance peaks (oscillations) which are associated with the formation of quantum well states in the middle metal layer 3 [8, 9, 11, 16, 19–22]. The period of these oscillations is the same for both curves and proportional to π/k_{E_F} (see, for example, ref. [11]), but the positions (phases) of the resonant peaks are shifted with respect to each other. The phase is defined by the boundary conditions at the metal/oxide interfaces. In the case of asymmetric double-barrier structures, the matching of the phases at the interfaces is sensitive to the direction of the current due to different D_{22} and D_{44} in (2) which depend exponentially on the barrier parameters leading to asymmetric voltage drops V_2 and V_4 . The difference in these voltage drops will bring the quantum well states in M_3 to line up differently with respect to the energy E of the electron under positive and negative applied voltage. The resulting phase shift of the current density leads, thus, to a current asymmetry ratio (forward current divided by reverse current and vice versa) which oscillates with the same period as the current density and which is considerably enhanced at its maxima. This oscillation of the asymmetry ratio as a function of b is shown in fig. 2(b). Hence, choosing the appropriate parameters of the layer thicknesses and the barrier heights, the asymmetry can be enhanced significantly (more than one order of magnitude), leading to the I - V characteristics presented in fig. 1(b), reminiscent of a diode. Similar characteristics were found for double-barrier structures with the same barrier heights but different barrier thickness. In contrast, for a symmetric double-barrier structure ($U_2 = U_4$ and $a = c$), the phase shift in the forward and reverse current densities is zero, resulting in a symmetric I - V curve for positive and negative applied voltage. Consequently the diode behavior is lost.

Replacing in the asymmetric double-barrier structure the outer layers M_1 and M_5 by ferromagnetic metals, it is found that the diode efficiency can be controlled by an applied magnetic field. Furthermore, it is found that the tunneling magnetoresistance (TMR) ratio itself depends strongly on the direction of the current yielding a high asymmetry ratio. The current density of such a magnetic double-barrier structure was calculated for the case of identical magnetic layers using Fermi wave vectors $k_{E_F}^\uparrow = 1.09 \text{ \AA}^{-1}$ and $k_{E_F}^\downarrow = 0.42 \text{ \AA}^{-1}$, which correspond to the spin-split free-electron-like d -electron bands of Fe [23]. The parameters for the other layers are the same as for the non-magnetic case discussed above. The TMR ratio

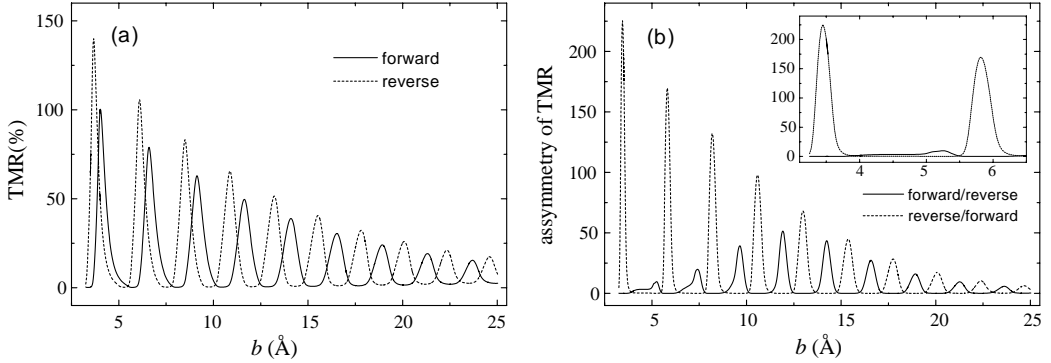


Fig. 3 – Dependence of (a) the TMR ratio and (b) its corresponding asymmetry ratio on b calculated from the forward and reverse current through an asymmetric double-barrier structure with magnetic outer layers (see text).

is defined as

$$\text{TMR} = \frac{\sum_{\sigma} (j_{\text{p}}^{\sigma} - j_{\text{ap}}^{\sigma})}{\sum_{\sigma} j_{\text{ap}}^{\sigma}},$$

where $j_{\text{p(ap)}}^{\sigma}$ is the current with spin σ for parallel (antiparallel) alignment of the magnetizations in the magnetic layers. In fig. 3(a) this TMR ratio is presented for an asymmetric structure with different barrier heights as a function of the thickness b . The TMR ratio reflects the oscillations of the current density as well as the phase shift between the forward and reverse bias (compare fig. 2). It follows that the TMR ratio is also very asymmetric and the corresponding asymmetry ratio can reach values up to 200 (fig. 3(b)) at the appropriate thickness b .

This TMR asymmetry leads to a “magnetically controlled” diode, whose blocking efficiency can be varied by a magnetic field. To illustrate this, we calculate the value of relative magnetoasymmetry (RMA)

$$\text{RMA} = \frac{\left(j_{\text{p}}^{\text{dir(inv)}} / j_{\text{p}}^{\text{inv(dir)}} \right) - \left(j_{\text{ap}}^{\text{dir(inv)}} / j_{\text{ap}}^{\text{inv(dir)}} \right)}{\left(j_{\text{ap}}^{\text{dir(inv)}} / j_{\text{ap}}^{\text{inv(dir)}} \right)}, \quad (3)$$

where $j_{\text{p}}^{\text{dir(inv)}}$ and $j_{\text{ap}}^{\text{dir(inv)}}$ are the total forward (reverse) current for parallel and antiparallel configuration of the magnetization, respectively. In fig. 4 the dependence of the RMA is shown as a function of b for the double-barrier structure of fig. 3. At the maxima the magnitude of the asymmetry ratio can be doubled by applying a magnetic field.

It is noted that much higher asymmetries can be obtained when the scattering in the metallic layers is weak. However, in this case the resonance peaks become narrow and are therefore more difficult to detect experimentally. More realistic is the case of strong scattering which leads to a broadening of the resonance peaks and consequently reduces the asymmetry ratios, with the advantage of being easier to detect experimentally. More critical for possible experimental observation of the predicted diode behaviour are barrier and metallic spacer thickness fluctuations. Further calculations show that thickness fluctuations which do not extend over two atomic layers preserve the quantum well states. Details of this work will be published elsewhere. As a final point we would like to underline that the general expressions (2) describes properly *both* ballistic and diffuse tunneling regime through the system.

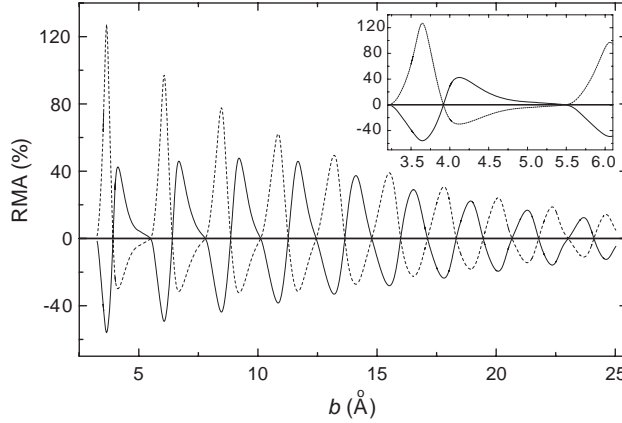


Fig. 4 – The relative magnetoasymmetry (RMA) as a function of the thickness b for the same asymmetric double-barrier structure as for fig. 3. The RMA is calculated from expression (3) with the current asymmetry ratio defined as $(j_{p(ap)}^{\text{dir}}/j_{p(ap)}^{\text{inv}})$ (solid line) and $(j_{p(ap)}^{\text{inv}}/j_{p(ap)}^{\text{dir}})$ (dashed line).

The transition from one regime to another can be retrieved if the scattering in the middle metallic layer M_3 is zero ($k_{E_F3}l_3 \rightarrow \infty$). In this case, the problem can be solved exactly and the analytic expressions in (2) yield that all tunneling probabilities are equal ($D_{ij}^\sigma = D^\sigma$ for $i, j = 2, 4$) so that the current density can be written as

$$j^\sigma = j_2^\sigma = j_4^\sigma = \frac{e}{\pi h} \int dE [f(E) - f(E + eV_{\text{ext}})] \int D^\sigma(E, \kappa) \kappa d\kappa$$

and the condition of constant current across the whole double-barrier structure is automatically fulfilled. This result means that in the case of an ideal structure without scattering, the purely quantum-mechanical problem of electron tunneling through the *entire* double-barrier structure is solved exactly describing the direct coherent process. In this case, the voltage drop in each barrier is proportional to its thickness as in refs. [8] and [9]. This remarkable result is important since it directly shows how the scattering in the middle layer destroys the direct ballistic process so that the tunneling across the structure is not described anymore by a single transmission matrix but by resistors in series. Moreover, it means that expression (2) can be written in the form

$$j_{2(4)}^\sigma = \frac{e}{\pi h} \int dE [f(E) - f(E + eV_{\text{ext}})] \int D_{24(42)}^\sigma(E, \kappa) \kappa d\kappa + \frac{e}{\pi h} \int dE [f(E_1) - f(E_2)] \int [D_{22(44)}^\sigma(E, \kappa) - D_{24(42)}^\sigma(E, \kappa)] \kappa d\kappa, \quad (4)$$

where $E_1 = E$, $E_2 = E + eV_2$ for j_2 and $E_1 = E + eV_2$, $E_2 = E + eV_{\text{ext}}$ for j_4 . The first term in (4) describes the direct ballistic process across the structure and the second one describes local processes which appear only in the presence of the scattering in the middle metallic layer.

In conclusion, we presented a quantum theory of the tunnel magnetoresistance in magnetic double-barrier structures and predicted a strong “diode”-like behaviour for the I - V characteristics and the TMR in the case of asymmetric barriers. It was shown that the asymmetry ratio can be controlled by an applied magnetic field. This phenomenon is due to the different phase shift of the quantum well states in the middle metal layer under forward and reverse applied voltage. This structure should have an important application as a blocking device in a MRAM.

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- [23] STEARNS M. B., *J. Magn. & Magn. Mater.*, **5** (1977) 167. The choice of free-electron-like parameters is justified by *ab initio* calculations of the spin-dependent tunneling with ferromagnetic 3d-metallic electrodes taking into account real electronic structure (MCLAREN J. M. *et al.*, *Phys. Rev. B*, **56** (1997) 11827; BUTLER W. H. *et al.*, *Phys. Rev. B*, **63** (2001) 054416). It was shown that most of the tunneling current is carried by hot spots in κ -space (in our case, the vicinity of $\kappa = 0$). This means that these electrons have a well-defined perpendicular component of the momentum which defines the period of the current oscillations *vs.* thickness *b*.