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Influence of quantum well states on transport properties of double barrier junctions

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Abstract

A strong asymmetric behavior in the I–V characteristics and the tunnel magnetoresistance in asymmetric magnetic double-barrier junctions is predicted. This effect relates to formation of quantum well states in the middle metallic layer. The influence of the random fluctuations of the barrier and the middle metallic layer thickness on the statistics of resonant levels is investigated. © 2002 Elsevier Science B.V. All rights reserved.

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Tunneling of spin-polarized electron through magnetic tunnel junctions (MTJ) has been attracting attention since high resistance and field sensitivity make them good candidates for use as high-density storage media and as field sensors. In most of the experiments, MTJ consist of two ferromagnets separated by an insulator (FM/I/FM) [1]. Another subject of high interest is multiple tunnel structures with two or more barriers since they can have considerably enhanced Tunnel magneto resistance (TMR) effect with a surprising weak decay of magnetoresistance with applied bias voltage [2]. In this paper, we present results of theoretical investigation of transport properties in asymmetric double barrier structures of the form $M_1/O_2\ a/M_3\ b/O_4\ c/M_5$ (a, b and c are the thicknesses of the corresponding layers). 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 ith metal. The outer metallic layers are assumed to be semi-infinite. In the case of symmetric structures with $a = c$ and $U_2 = U_4$ [3,4], 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 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 [5]. Here, D is derived using the Green functions technique in the mixed real space–momentum representation [6,7] and can be written in the form

$$D = \frac{4}{\pi}\frac{e^2}{\hbar}\left(\frac{\hbar^2}{2m}\right)^2 \sum A_\kappa(z,z')\,\overleftrightarrow{\nabla}_z\,\overleftrightarrow{\nabla}_{z'}A_\kappa(z,z'), \tag{1}$$

where $\overleftrightarrow{\nabla}_z = (1/2)(\overrightarrow{\nabla}_z - \overleftarrow{\nabla}_z)$, $A_\kappa(z,z') = (\mathrm{i}/2)\{G_\kappa^{\mathrm{ret}}(z,z') - [G_\kappa^{\mathrm{ret}}(z,z')]^*\}$ with retarded and advanced Green functions, z is the coordinate perpendicular to the plane of the structure. 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. By solving the Schrödinger equation in each layer and matching the boundary conditions at the interfaces, we have found the Green function (see Ref. [8] for details). From the Green function, the

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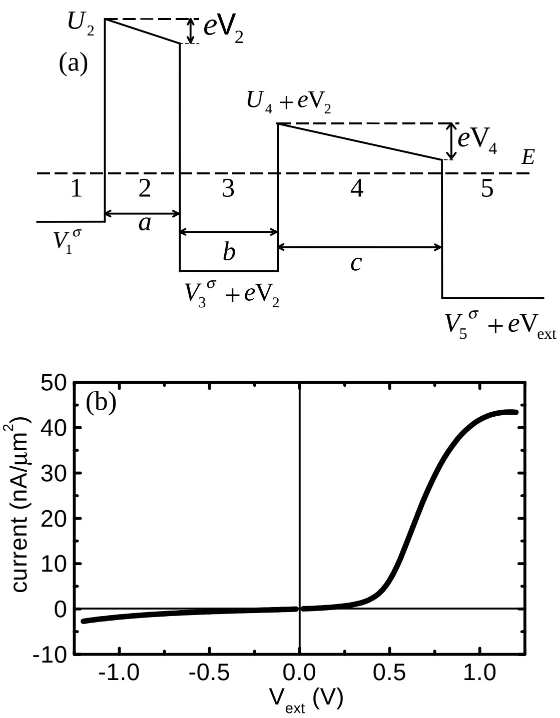

Fig. 1. (a) Potential energy diagram and (b) the calculated current–voltage curve for the asymmetric structure Cu/O_2 7 Å/Cu 5.5 Å/O_4 21 Å/Cu with $U_2 - E_F = U_4 - E_F = 3$ eV.

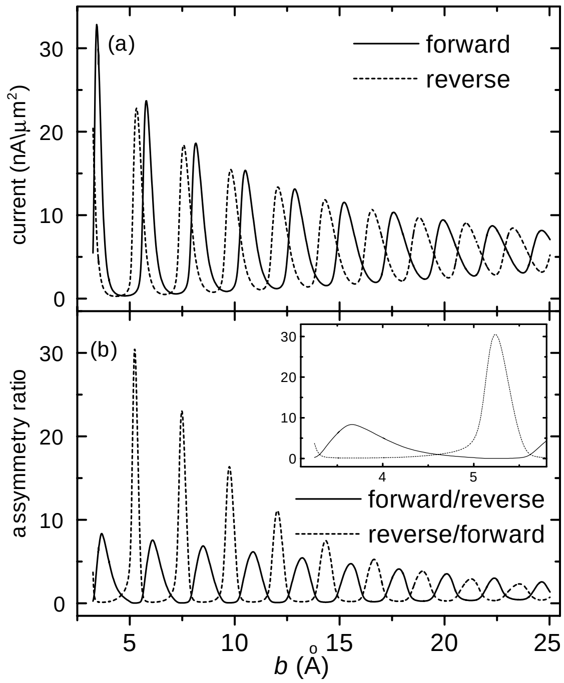

Fig. 2. Dependence of (a) the forward and reverse current and (b) the corresponding asymmetry ratio on the layer thickness b of the middle metallic layer for the non-magnetic asymmetric double barrier structure (see text).

non-local probability D is calculated using formula (1) [8]. 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 [6] (see Fig. 1(a)). This yields the four analytical expressions: D_{22}, D_{24}, D_{42} and D_{44}. 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 [5,8]:

$$
\begin{aligned}
j^\sigma_{2(4)} = &\frac{e}{\pi h}\int \mathrm{d}E[f(E) - f(E + eV_2)] \int D^\sigma_{22(42)}\kappa\,\mathrm{d}\kappa \\
&+ \frac{e}{\pi h}\int \mathrm{d}E[f(E + eV_2) \\
&- f(E + eV_{\mathrm{ext}})] \int D^\sigma_{24(44)}\kappa\,\mathrm{d}\kappa, \qquad (2)
\end{aligned}
$$

where $f(E)$ is the thermal occupation probability of a state with energy E. Finally, from the requirement that the current density has to be constant throughout the whole barrier structure, $j_2^\sigma = j_4^\sigma$, 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 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. 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 $V_{\mathrm{ext}} = 0.7$ V for a double barrier structure of Cu/$O_2$21 Å/Cu b Å/O_4 21 Å/Cu [8] with different barrier heights ($U_2 - E_F = 1$ eV and $U_4 - E_F = 3$ 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 [3,4,6]. The period of these oscillations is the same for both curves and proportional to π/k_{E_F} (see, for example, Ref. [6]), 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 Eq. (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 (Fig. 2(b)). Hence, by 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 thicknesses. Replacing the outer layers M_1 and M_5 in the asymmetric double-barrier structure by ferromagnetic metals, it is found that the diode efficiency can be controlled by an applied magnetic field. Furthermore, it is found that the TMR ratio itself depends strongly on the direction of the current yielding a high asymmetry ratio [8]. 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. The barrier and metallic spacer thickness fluctuations are more realistic and critical for possible experimental observation of the predicted diode behaviour. To investigate the influence of the random fluctuations of the barrier and the middle metallic layer thickness on the statistics of resonant levels, we assume that the thickness of the layers can vary by an integer number, n, of atomic planes around its average value. Furthermore, the thickness fluctuations occur on the finite areas, S_i ($i = 1, \ldots, n$), of the cross section of the structures forming the lateral terraces (S_0 is the area of main terrace corresponding to thickness b). In Fig. 3, we plotted the total current through the structure as well as the contribution to it from all terraces for the case $n = 2$. One can see that thickness fluctuations strongly affect the quantum well states smearing the oscillations in the total current.

As a final point, we would like to underline that the general expressions (2) describe properly *both* the coherent and non-coherent tunneling regime through the system. The transition from one regime to another can be retrieved if the scattering in the middle metallic layer M_3 is zero. In this case, the problem can be solved

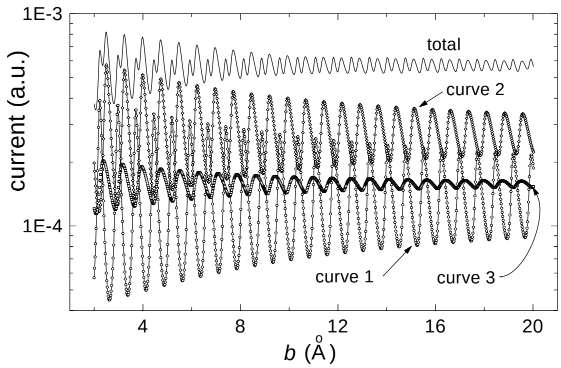

Fig. 3. The total current through the double barrier junction and contribution to it from the main terrace with $S_0 = 10\,000$ Å (curve 1) and "hot spots" with $S_1 = 1000$ Å (curve 2) and $S_2 = 100$ Å (curve 3) as a function of the average thickness b.

exactly and the analytic expressions in (2) yield that all tunneling probabilities are equal ($D^{\sigma}_{ij} = D^{\sigma}$ for $i,j = 2,4$) 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. [3,4].

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