Spin-dependent transport in a double barrier structure with a ferromagnetic material emitter

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Abstract

The differential conductance for a double barrier resonant tunnel diode is calculated by a recursive Green-function method based on the Keldysh formalism. The calculated results show that the conductance is strongly spin dependent for only the case where a positive bias voltage is applied between two barriers. The lifetime broadening at the Fermi level due to the magnetic impurity is found to be important to understand the dip structure of the conductance curve in experimental results. The features of the splitting of the dips in the calculated results are consistent with those in the experimental results. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The magnetic semiconductors (Ga–Mn)\textsubscript{As} and (In–Mn)\textsubscript{As} allow us to study the magneto-transport properties of layered systems grown epitaxially and the spin injection to semiconductors \cite{1,2}. These materials are known to be unique to show a high Curie temperature of 100 K or above. Many experimental and/or theoretical studies have been done \cite{3–6} to elucidate the origin of the ferromagnetism of these materials.

Even with these studies, however, understanding of the origin seems to be still in developing stages.

In the previous study, in order to clarify the origin of ferromagnetism, we have performed the band structure calculations of (Ga–Mn)\textsubscript{As}, and have shown that the Mn dopant can cause strong disturbance on the electronic structure near the valence band where the Fermi level can exist \cite{7}. Because of the ferromagnetism of these materials, the disturbance on the electronic structure is naturally spin dependent. Such a strong perturbation on the electronic states at the top of valence band is expected to affect the transport properties.
Using these results, in this study, we have calculated the transport properties for a double barrier resonant tunnel diode (RTD) with a ferromagnetic emitter, to justify the validity of these results in real concentrated systems. Recently, magneto-tunneling properties of RTD’s can reveal a number of interesting phenomena related to tunneling in semiconductors [8–11]. For example, magneto-tunneling properties of AlAs/GaAs/AlAs double barrier RTD with ferromagnetic p-type (Ga,Mn)As have been examined experimentally [10,11]. In that study, the resonant dip splitting has been observed below the ferromagnetic transition temperature of (Ga–Mn)As without magnetic field [10,11]. For the RTD structure, we have used a microscopic model which can be applicable to the complex structure of the sample geometry under finite bias voltages. The method employed is based on Keldysh’s theory, and is an extension of the recursive Green function method for a lattice model [12].

Using this model, we have attempted to reproduce qualitatively the main features in the experimental results [10,11], although quantitative treatments for the band structure of the real materials have not been done in this study.

2. Model and method

We consider a multilayer structure, in which the parameter $l$ is introduced as a label of the layer in $z$-direction (stacking direction). The regions where $l \leq 0$ and $l \geq N + 1$ are the semi-infinite leads and the region where $1 \leq l \leq N$ is the central region containing the double barriers. The thickness of the barrier layer is $2a$ with $a$ being the lattice constant and the cross section of the system is $Ma \times Ma$. The periodic boundary conditions are adopted in the $x$- and $y$-direction. The parameters $N$ and $M$ are set to be twelve and three in this work, respectively. The Hamiltonian $\mathcal{H}$ is given by

$$
\mathcal{H} = -t \sum_{\langle i,j \rangle \langle \ell,\ell' \rangle, \sigma} (c_{i,\ell,\sigma}^\dagger c_{i',\ell',\sigma} + \text{h.c.}) + \sum_{i,\sigma} V_{i,\sigma}(r_i) c_{i,\sigma}^\dagger \int c_{i,\sigma} + \sum_{\ell,\sigma} l=1 \sum_{l=1}^N (\Phi_l + V^l_{\ell,\sigma}) c_{i,\ell,\sigma}^\dagger c_{i,\ell,\sigma},
$$

where $r_i$ denotes the positional vector in $x$–$y$ planes, $c_{i,\ell,\sigma}^\dagger$ is the creation operator for a hole at the site $(r_i, l)$ with spin $\sigma$, $t$ is the nearest-neighbor transfer integral, and $V_{i,\sigma}(r_i)$ is the potential energy. In the last term, $\Phi_l$ appears when the bias voltage $V$ along the $z$-direction is applied to outside of the central region, and we assume the electrostatic potential to be $\Phi_l \equiv eV$ in the left lead, and $\Phi_l \equiv 0$ in the right lead. For $1 \leq l \leq N$, it is assumed to be $\Phi_l = eV(N + 1 - l)/(N + 1)$ when the electric field is uniform. We take the chemical potential of the left and right leads, $\mu_L$ and $\mu_R$, to be $\mu_L = \mu_R + eV$. The quantity $V^l_{\ell,\sigma}$ is the on-site energy of the double barrier. The total current flowing along the $z$-direction can be obtained by the method described in Refs. [12,13].

The detailed description for the calculation of the interlayer Green’s function is also given in Ref. [12].

3. Results and discussion

Now we discuss the transport phenomena through the double barrier region. We are concerned with a hole transport, considering the hole transport occurring in the experiment of RTD with p-type (Ga–Mn)As or p-type GaAs as an emitter material [10]. In the present study, we take the transfer integral $t$ as a unit of the energy. On the basis of the comparison between the valence band width of GaAs ($\sim 4.3$ eV for a light hole) and that of the tight-binding model $12t$, the value $1.0t$ used in this study may correspond to about 0.36 eV. Here, we describe the parameters employed in this study briefly. The chemical potential in the right lead $\mu_R$ is set to be $\mu_R = -5.8t$ ($\mu_L = \mu_R + eV$). The values of $\mu_R$ and $\mu_L$ correspond to be $0.2t$, if we measure the chemical potentials from the bottom of the band. Inside the double barrier ($1 \leq l \leq 2, 11 \leq l \leq 12$), $V^l_{\ell,\sigma}(r_i)$ is chosen to be the barrier height $1.0t$. At the left lead wire ($l \leq 0$), $V_{i,\ell,\sigma}(r_i)$ is taken to be $\pm(5/3)E_{\text{ex}}$ with $E_{\text{ex}}$ being the exchange energy. For another region ($l \geq 1$), $V_{i,\ell,\sigma}(r_i)$ equals zero. From the previous study [7], we have considered an effective exchange splitting $E_{\text{ex}}$ caused by the presence of the finite number of holes and the broadening of the resonant state at the top of the valence band in the real concentrated system [7]. In practice, the effective splitting can be estimated from the experimental results [10].
We have calculated the differential conductance estimated from the total current. Fig. 1 depicts the bias voltage dependence of the differential conductance $dI/dV$ for various temperatures. As a remarkable feature in Fig. 1, we can see sharp peaks and dips in the conductance curve, at $k_B T = 0$ with $k_B$ being the Boltzmann constant. Also, one can easily notice the splitting of dips, despite the absence of the splitting of peaks. First, we discuss the appearance and temperature dependence of the peaks and dips in the conductance curves in Fig. 1. These peaks are considered to occur when $\mu_L$ crosses the local energy level constructed in between the two barriers as $eV$ increases, and these dips appear when the bottom of the first sub-band for the left lead crosses the local energy level. In other words, the peaks (dips) occur when one level enters (leaves) the energy range contributing to the current, i.e., $\mu_R < E < \mu_L$ at $T = 0$. As the temperature increases, the sharp peaks become broader because of the broadening of the Fermi surface, although the change of the shape of dips is small (see Fig. 1). In the experiment [10,11], there appears no peak in the differential conductance curve, and the shape of the curve seems to resemble the structure of the curve shown in Fig. 1 at $k_B T = 0.2$. Thus, we can understand that the broadening of the Fermi surface is significant for explaining the dip structure of the $dI/dV$ curve in the experimental results [10]. In the real materials we treat in this study, the life time broadening at the Fermi level due to the magnetic impurities is important, rather than the effect of real temperatures, and then, we assume that in the present study, the life-time broadening can be replaced with temperature broadening $k_B T = 0.2t$ for simplicity. Here, for justifying the validity of this value of broadening, we calculated the self-energy by using CPA. The random potentials for $\uparrow$ and $\downarrow$ spin electrons estimated in the previous study [7] are $\sim 1.9t$ and $\sim 3.5t$, respectively. The CPA calculation gives the imaginary parts of the self-energy of $\uparrow$ and $\downarrow$ spin states $\sim -0.05t$ and $\sim -0.4t$, respectively. The magnitude of the self-energy broadening calculated by CPA is the same order of the value of the broadening estimated from the calculated conductance curves shown in Fig. 1. In what follows, we take the value $k_B T = 0.2t$ as the life-time broadening.

Next, we discuss the splitting of dips in Fig. 1. As described before, the dip appears when the bottom of the first subband for the left lead crosses the local energy level, so that the splitting of dips occurs by the exchange splitting of the subband. However, the peaks never split because of little influence on the Fermi level ($\mu_L$) by the exchange splitting of the sub-band. To see these features of splitting of the dip more clearly, we have calculated the $eV$-dependence of the differential conductance for various $E_{\text{ex}}$, and the results are shown in Fig. 2. The magnitude of the splitting of the dip increases with increasing $E_{\text{ex}}$ linearly, and the value of the splitting is half the magnitude of $E_{\text{ex}}$ (see Fig. 2). The value $E_{\text{ex}} \sim 0.2t$ (with $t \sim 0.36$ eV) accords with the experimental result [10,11]. It should be noted that the higher the bias voltage varies, the broader the dips become. Consequently, the splitting can be seen clearly in a lower rather than in a higher bias voltage region. This characteristic can be in agreement with the experiment [10,11], where the dips in the higher bias-voltage region never split into two. Moreover, the magnitude of the left hand side dip in each splitting dips is larger than that in the right hand side dip. This is due to the following reasons. The left dip corresponds to the resonance of the $\uparrow$ spin state in which the bottom of the subband shifts to up from that in the $\downarrow$ spin state by $E_{\text{ex}}$. Accordingly, the amount of the local state in the energy region contributing to the current for $\downarrow$ spin state is larger than that for the $\uparrow$ spin state, and hence, the $\uparrow$ spin state is
more sensitive to the phenomenon that a single energy level emerges from the region contributing to the current. In addition, for an incident hole, with increasing energy, relative height of the double barrier decreases, so that the local level is broadened for the resonance of the $\downarrow$ spin state rather than for that of the $\uparrow$ spin state.

Furthermore, we can also notice the presence of small dip at $eV = 0.2t$ and $E_{ex} = 0$ in Fig. 2. This dip splits into two at $E_{ex} = 0.08t$, but at $E_{ex} = 0.16t$, the left side dip disappears (see Fig. 2). This is because the energy level corresponding to the left dip lies below the bottom of the first subband even at the case where the bottom of the first subband in the left lead coincides with $\mu_R$ for $E_{ex} = 0.16t$. This feature may be consistent with the lack of splitting of HH1 dip in Ref. [10,11].

So far, we have shown the calculated results where the bias voltage applied is positive. As described before, the splitting of the dip is due to the exchange splitting of the bottom of the subband only in the left hand side region. Therefore, we can expect that the splitting hardly occurs for the case where the bias voltage is applied reversely, i.e., the bias voltage applied is negative. We have examined the effect of the inversion of the bias voltage on the differential conductance. Fig. 3(a) displays the example of the calculated conductance where the negative bias voltage is applied to

the central region, i.e., $\mu_L = \mu_R - eV$ in this case. We also show the conductance in the case of positive bias voltage in Fig. 3(b) as a reference. In these figures, we draw the conductance for $\downarrow$ and $\uparrow$ spin states independently. As can be seen from Figs. 3(a) and (b), as we would expect, only in the case for the positive bias voltage applied, the dips for both spin states appear separately. These calculated results are in agreement with the experimental results [10,11].

4. Summary

In summary, we have calculated the differential conductance for a double barrier resonant tunnel diode with a ferromagnetic material as an emitter. We have employed the recursive Green-function method based on the Keldysh formalism. We have found that the conductance is strongly spin dependent for only the case where a positive bias voltage is applied between two barriers. Also, it has been found that the life time broadening at the Fermi level due to the magnetic impurity is important to understand the dip structure of the conductance curve in the experimental results. The effect of the life time broadening on the conductance
is included in the calculation in terms of the effect of a temperature. The features of the behavior of dips in the conductance curve reported can be reproduced qualitatively by these calculations.

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