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11 June 2001

PHYSICS LETTERS A

Physics Letters A 284 (2001) 205–215

www.elsevier.nl/locate/pla

Quantum size effect and temperature effect on spin-polarized transport in $ZnSe/Zn_{1-x}Mn_xSe$ multilayers

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Received 9 November 2000; received in revised form 2 April 2001; accepted 26 April 2001
Communicated by A. Lagendijk

Abstract

We present tight-binding Green's function investigations of the influence of quantum sizes and the temperature on spin tunneling transport through a tunable $ZnSe/Zn_{1-x}Mn_xSe$ multilayers under an external electric field. It is found that the degree of polarization can be significantly induced by the size of the corresponding structure. As the size of the multilayers is increasing, both the transmission spectra and the current density spectra become more complicated and the degree of spin polarization is higher. It is also found that the degree of the spin polarization is drastically reduced as the temperature is increasing. © 2001 Elsevier Science B.V. All rights reserved.

PACS: 75.50.Pp; 72.10.-d; 72.90.+y; 84.32.-y
Keywords: Spin polarization; Tunneling; Heterojunctions; Semimagnetic semiconductor

1. Introduction

Recently there has wide-spread study of the phenomena of spin-polarized transport and the development of device applications [1–8]. In the applications, the spin of the electron has been taken into consideration for the design of new quantum devices, such as spin quantum computers [1], spin-memory devices [2], spin transistors [3], spin filters and modulators, etc. Single spin is considered as the ultimate limit of information storage [4]. However, none of these devices exist yet, and experimental progress as well as theoretical investigation are needed to provide guidance and support in the search for realizable implementations. The first active device was suggested by Datta and Das in 1990 [5]. They proposed a transistor utilizing spin-dependent effects in a two-dimensional electron gas contacted with two ferromagnetic electrodes. Most of the proposed spintronic devices involve spin-polarized transport across interfaces in various hybrid structures. To determine the feasibility of spintronic devices and more generally of various applications of spin-polarized transport, it is essential to answer questions like how to create and detect spin-polarized carriers and how to maintain their spin polarization and spin coherence for relatively long times.

Spin-superlattice was theoretically proposed by von Ortenberg [9] and experimentally realized by Dai

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PII: S0375-9601(01)00285-7

et al. [10] and Chou et al. [11], respectively. After that many creative theoretical and experimental works have been done by exploiting spin-dependent phenomena. Studies on spin-polarized transport are growing dramatically in number, especially for ferromagnetic metal [4], magnetic tunnel junctions [12], diluted magnetic semiconductor heterostructures [13], ferromagnetic semiconductor heterostructures [14], semiconductor–superconductor hybrid structures [15], etc. Sugakov and Yatskevich [16] examined spin splitting in parallel electric and magnetic fields through a double-barrier heterojunction using transfer-matrix method. Recently, Carlos Egues [17] theoretically investigated electronic spin filtering in perpendicular transport through a tunable $ZnSe/Zn_{1-x}Mn_xSe$ heterostructure with single paramagnetic layer. The results indicate a strong suppression of the spin-up component of the current density while increasing magnetic fields and the total current density is dominated by the spin-down component for $B > 2$ T. The reason is that in an external magnetic field the paramagnetic layer of the heterostructure behaves as a potential well for spin-down electrons and a potential barrier for spin-up ones. The study has shown that the electric field can greatly change the status of polarization of the tunneling electron in $ZnSe/Zn_{1-x}Mn_xSe$ heterostructures with single paramagnetic layer [18]. Further, interesting spin resonant suppression and enhancement are found in semimagnetic semiconductor heterostructures with double paramagnetic layers, which are originated from the combined effects of the structural asymmetry and the external fields [19].

It is known that electric multiple-barrier or electric multiple-well structures possess superior features over electric single-barrier or single-well structures in many aspects. Therefore, it is expected that the $ZnSe/Zn_{1-x}Mn_xSe$ multilayered heterostructures with two or more paramagnetic layers possess some novel spin-dependent features. In this Letter we adopt the method of tight-binding Green's function and investigate the influence of quantum sizes and the temperature on the spin-polarized transport through $ZnSe/Zn_{1-x}Mn_xSe/ZnSe/Zn_{1-x}Mn_xSe/ZnSe$ multilayers under both an electric field and a magnetic field. We find that the degree of polarization of electron beams can be markedly tuned by adjusting the size of the corresponding system as well as by the temperature. We also present investigations of the local density of states (LDOS), through which spin-dependent tunneling features found in the considered system are reasonably illustrated.

2. Method of tight-binding Green's function

In Mn-based semimagnetic semiconductor systems electrons interact with the 3d electrons of the localized magnetic moments of the Mn ions via the sp–d exchange interaction. For a conduction electron, this exchange interaction can be written as Heisenberg type Hamiltonian

$$H_{\text{int}} = -\sum_i J\left(\vec{r} - \vec{R}_i\right)\vec{S}\cdot\vec{S}_i, \tag{1}$$

where $\vec{r}$ and $\vec{S}$ are the position and the spin of the conduction electron, R_i and S_i are positions and spins of i numbers Mn^{2+} ions, respectively. Within typical approximations, it allows to calculate energy states of conduction and valence electrons by $k \times p$ perturbation method. The $k \times p$ matrix is augmented by diagonal terms which for the conduction band are equal to $A = N_0\alpha\sigma_z x\langle S_z\rangle$, where N_0 is the number of units cells per unit volume, $\alpha = \langle\Psi|J|\Psi\rangle$ is the exchange integral, parameter of interaction of electrons with Mn^{2+} ions, σ_z is the electron spin components $\pm 1/2$ (or $\uparrow, \downarrow$) along the field, x is the mole fraction of Mn, and $\langle S_z\rangle$ is the thermal average of zth component of Mn^{2+} spin (a $5/2$ Brillouin function).

Because of the sp–d exchange interaction, an external magnetic field applied to the $ZnSe/Zn_{1-x}Mn_xSe$ system with multiple paramagnetic layers modulates the potential profile seen by a traversing electron (or heavy hole) in a spin-dependent fashion. Spin-down electrons see a multiple-well potential while spin-up ones see a multiple-barrier potential. In this section, we constrict our theoretical analyses to the $ZnSe/Zn_{1-x}Mn_xSe/ZnSe/Zn_{1-x}Mn_xSe/ZnSe$ multilayers with two $Zn_{1-x}Mn_xSe$ paramagnetic layers. The formalism obtained can be naturally extended to the structure with more paramagnetic layers. Within mean field and for a magnetic field along the z axis, the sp–d exchange interaction gives rise to a spin-dependent potential

$$V_{\sigma_z} = -N_0\alpha\sigma_z x\langle S_z\rangle$$

$$\times\big[\Theta(z)\Theta(L_1-z) + \Theta(z-L_1-L_2)\Theta(L_1+L_2+L_3-z)\big] \tag{2}$$

in the Hamiltonian of the system. Here, $\Theta(z)$ is the Heaviside function, L_1 and L_3 are the widths of left and right $Zn_{1-x}Mn_xSe$ paramagnetic layers, and L_2 is the width of the ZnSe layer between the two paramagnetic layers. Under an applied bias V_a along the z axis, an electric-field-induced term $-eV_az/L_t$ ($L_t = L_1+L_2+L_3$) should be added to the potential. The Hamiltonian of an electron in the framework of the parabolic-band effective-mass approximation can be written as

$$\hat{H}_{xy} = \frac{1}{2m_e^*}\big[\hat{P}_x^2 + \big(\hat{P}_y + eBx\big)^2\big], \tag{3}$$

$$\hat{H}_z = \frac{1}{2m_e^*}\hat{P}_z^2 + V_{\sigma_z}(z) - \frac{eV_az}{L_t}. \tag{4}$$

In the absence of any kind of electron scattering the motion along the z axis is decoupled from that of the x–y plane. The in-plane motion is quantized in Landau levels with energies $E_n = (n+1/2)\hbar\omega_c$, where $n = 0, 1, 2, \ldots$ and $\omega_c = eB/m_e^*$ (we assume a single electron mass m_e^* throughout the heterostructure). Therefore, the motion of the electrons can be reduced to one-dimensional problem along the z axis. In the following we present numerical results of local density of states, the transmission coefficient, and the current density by using the method of tight-binding Green's function. The latter two physical quantities can also be determined from the standard transfer-matrix method [20]. We find that the numerical results obtained by using Green's function are well coincided with that by using transfer-matrix method. In the present Letter we do not want to present detail comparison. The key point here is that we can easily determine the local density of states by using method of tight-binding Green's function, which can be used to help us to understand the results obtained in this work.

Within the tight-binding formalism, we can model the reduced one-dimensional motion in ZnSe/$Zn_{1-x}Mn_xSe$ multilayers by the following Hamiltonian:

$$H_z = \sum_{i\sigma_z}\varepsilon_{i\sigma_z}\alpha^\dagger_{i\sigma_z}\alpha_{i\sigma_z} - \sum_{ii'\sigma_z}V\alpha^\dagger_{i\sigma_z}\alpha_{i'\sigma_z}, \tag{5}$$

where the sum over lattice sites i and i' is restricted to nearest neighbors, $V = \hbar^2/2m_e^*a^2$ is the hopping integral and set its value equal to one as the energy unit.

The spin-dependent local density of states (LDOS) $\rho_{\sigma_z}(E_z; z)$ is related to the Green's function of a whole system via a standard formula

$$\rho_{\sigma_z}(E_z; z) = -\frac{1}{\pi}\lim_{\varepsilon\to 0^+}\operatorname{Im} G_{\sigma_z}(E_z + i\varepsilon; z, z). \tag{6}$$

This expression allows the LDOS to be calculated as a function of the electron energy E_z as well as the space coordinate z for a system with multiple layers.

The transmission coefficients through the system can also be obtained from the Green's function as

$$\begin{aligned} T_{\sigma_z}(E_z, B, V_a) &= \frac{2a^2}{L_z^2}\operatorname{Tr}\big[\tilde{G}_{\sigma_z}(j, j')\tilde{G}_{\sigma_z}(j'-1, j-1) \\ &\quad + \tilde{G}_{\sigma_z}(j-1, j'-1)\tilde{G}_{\sigma_z}(j', j) \\ &\quad - \tilde{G}_{\sigma_z}(j, j'-1)\tilde{G}_{\sigma_z}(j', j-1) \\ &\quad - \tilde{G}_{\sigma_z}(j-1, j')\tilde{G}_{\sigma_z}(j'-1, j)\big], \end{aligned} \tag{7}$$

where $\tilde{G}_{\sigma_z}(j, j') = [G_{\sigma_z}(E_z + i\varepsilon; j, j') + G_{\sigma_z}(E_z - i\varepsilon; j, j')]/2i$ with G_{σ_z} is the matrix element of the real space Green's function. Note that the transmission coefficients are functions of the incident energy E_z, the magnetic field B, and the applied bias V_a.

We assume that the ZnSe layers are emitter and collector attached to external leads. The average spin-dependent current density is defined by

$$\begin{aligned} I_{\sigma_z}(B, V_a) &= e\sum_{n,k_y,k_z\geqslant 0} v_z(k_z)T_{\sigma_z}(E_z, B, V_a) \\ &\quad\times\left\{f\left[E_z + \hbar\omega_c\left(n+\frac{1}{2}\right)\right]\right. \\ &\quad\left. - f\left[E_z + \hbar\omega_c\left(n+\frac{1}{2}\right) + eV_a\right]\right\} \\ &\quad\times\int|\psi_{n,k_y,k_z}|^2\,dv, \end{aligned} \tag{8}$$

where

$$\psi_{n,k_y,k_z} = \frac{1}{\sqrt{L_y}}\frac{1}{\sqrt{L_z}}e^{ik_yy}e^{ik_zz}\varphi_n(x).$$

Here, $\varphi_n(x)$ is the nth harmonic-oscillator eigenfunction centered at $x_0 = -\hbar k_y/m\omega_c$, and k_y and k_z are the electron wave vectors along the y and z directions.

The summation on k_y is equal to $L_x L_y eB/2\pi\hbar$, $\varphi_n(x)$ is normalized. Therefore, Eq. (8) becomes

$$J_{\sigma_z}(B, V_a) = J_0 B \sum_{n=0}^{\infty} \int_0^{+\infty} T_{\sigma_z}(E_z, B, V_a) \times \left\{ f\left[E_z + \hbar\omega_c \left(n + \frac{1}{2} \right) \right] - f\left[E_z + \hbar\omega_c \left(n + \frac{1}{2} \right) + eV_a \right] \right\} dE_z, \quad (9)$$

where $J_0 = e^2/4\pi^2\hbar^2$.

3. Results and discussion

In this section we discuss spin-dependent tunneling transport through $ZnSe/Zn_{1-x}Mn_xSe$ multilayers with two paramagnetic layers. Electrons in Mn-based systems interact with the 3d electrons of the localized magnetic moments of the Mn ions via the sp–d exchange interaction. The concentration of Mn in the paramagnetic layer is chosen so that in the absence of an applied magnetic field, the conduction and valence band offsets are nearly zero. In an external magnetic field the sp–d exchange interaction gives rise to a giant spin splitting ΔE_s which exceed both the Landau level splitting $\hbar\omega_c$ and the thermal energy $k_B T$ [21], which lifts the degeneracy of the spin-up and spin-down electron and hole states. The paramagnetic layer in $ZnSe/Zn_{1-x}Mn_xSe$ multilayers behave as a well potential for spin-down electrons and a barrier potential for spin-up ones. Thus, in our considered multilayers, spin-up electrons see a double-barrier potential while spin-down ones see a double-well potential. When we adjust the widths of two paramagnetic layers, or apply an external electric field to the system, or change the strength of the applied magnetic field, the effective potential "seen" by electrons is changed correspondingly. Therefore, there should exist rich interesting spin-dependent tunneling features in our considered system.

Fig. 1 shows the spin-dependent transmission coefficients for electron traversing the $ZnSe/Zn_{1-x}Mn_xSe$ multilayers with different widths at zero bias and at an applied bias. Here we set $L_1 = L_2 = L_3 = L_0 = 10$, 50, 100 nm, respectively, and $B = 0.5$ T. In all of graphs, we use $m_e^* = 0.16m_e$ (m_e is the mass of free electron), an effective Mn concentration $x_{\text{eff}} = x(1 - x)$[12] with $x = 0.05$, $N_0\alpha = 0.26$ eV. The temperature is set to be $T = 4.2$ K in all of graphs of Figs. 1–4. In these cases, the magnetic-induced potential at zero bias is a symmetric double-well or double-barrier, so one can see unit quantum resonance for both spin-up and spin-down electrons. With increasing the width of the multilayers, the transmission spectra become more complicated, more resonant peaks with unity peak-value appear, and peaks become more sharper, especially in the low incident energy region. For spin-up electrons tunnel through the structure with larger size, there are several very sharp line-type peaks, within them the transmission is drastically suppressed, which is quite different from the spin-down case. In the latter, resonant peaks correspond to above-well virtual-state resonance in electric-well structures. At an applied bias, resonance in low energies is drastically suppressed due to the breakup of symmetry of the corresponding effective potential. Moreover, our numerical results also indicate that for electrons tunneling through the semimagnetic semiconductor heterostructure, unit transmission resonance is shifted to low energy region for larger L_2 of the middle ZnSe layer. Further, the spacing between adjacent resonant peaks narrows with increasing the widths of L_2. It is well known that both the quasibound state energies of a potential well and the spacing between adjacent quasibound energy levels are determined by the depth and width of the well. The wider is the width, the lower the eigenenergies of bound states are and the spacing between adjacent eigenstates is narrowed correspondingly. With these in mind, we can easily understand the above-stated size-dependent features.

Recently, there are several studies on spin transport in single or double electric-barrier structures [22–24] and in magnetic-barrier structures [20], the results indicated that there exists spin-dependent polarization for electrons. However, the degree of polarization is too much low than that found in the system considered here. The reason is that the effective potential of the $ZnSe/Zn_{1-x}Mn_xSe$ multilayers is quite different for spin down electrons and for spin up electrons: the potential for spin-up electrons is double barriers, while the potential for spin-down ones is double wells. Therefore, spin transport process shows

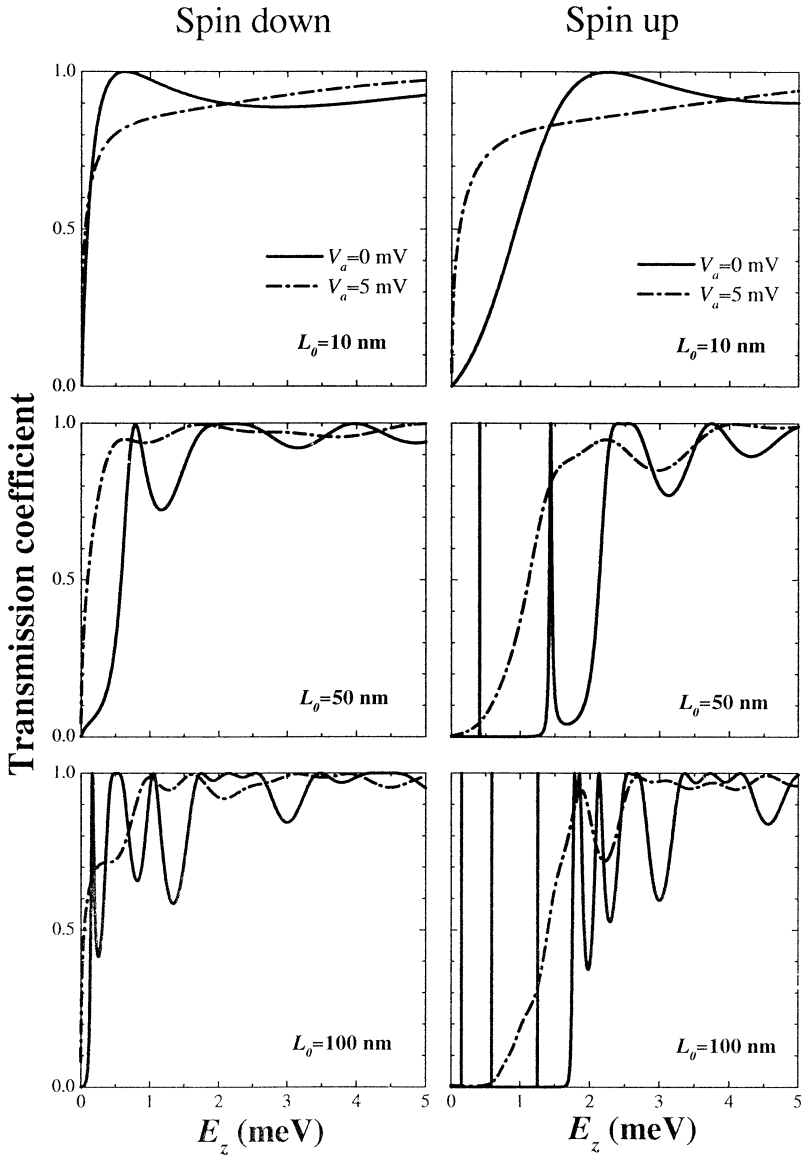

Fig. 1. Spin-dependent transmission coefficients for spin-up and spin-down electrons traversing $ZnSe/Zn_{1-x}Mn_xSe$ multilayers with different widths $L_0 = 10$, 50, 100 nm at zero bias and at an applied bias $V_a = 5$ mV. $B = 0.5$ T.

stronger spin-filtering properties in our considered system.

It is well known that many important physical properties and characteristics of a system with multilayers are determined by the density of states. In order to help readers better understand the spin-dependent features appeared in Fig. 1, in Figs. 2 and 3 we present LDOS distribution within the structure for $ZnSe/Zn_{1-x}Mn_xSe$ multilayers with widths $L_0 = 10, 30$ nm as the functions of the electron energy E_z and the space coordinate z, which illustrates the spatial localization over the structure. At zero bias, the states are almost completely localized inside the two wells for spin-down electrons, while for spin-up electrons the states also

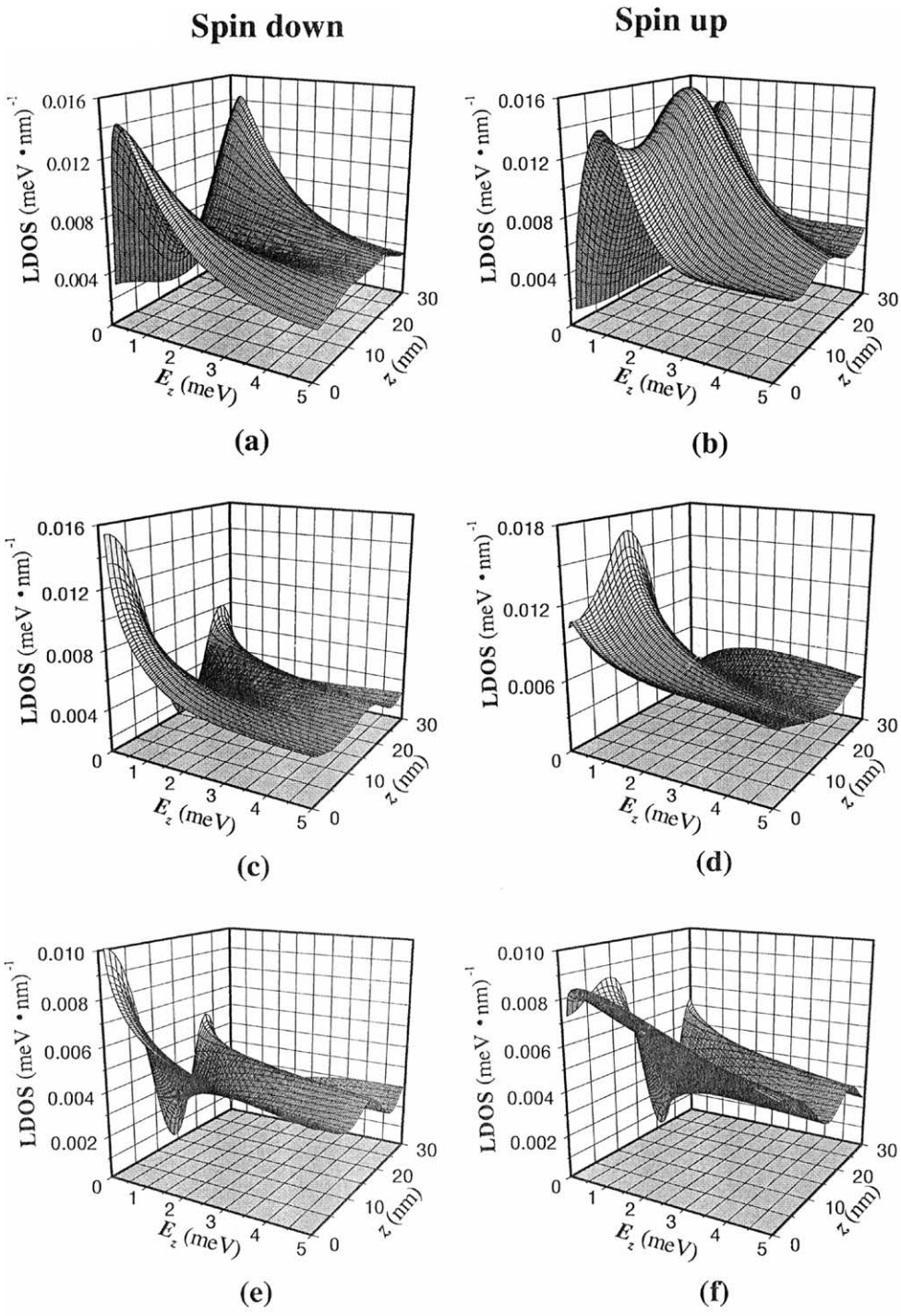

Fig. 2. LDOS distribution within $ZnSe/Zn_{1-x}Mn_xSe$ multilayers at zero bias and at applied biases. $L_0 = 10$ nm, $B = 0.5$ T. (a) and (b) $V_a = 0$ mV; (c) and (d) $V_a = 5$ mV; (e) and (f) $V_a = 10$ mV.

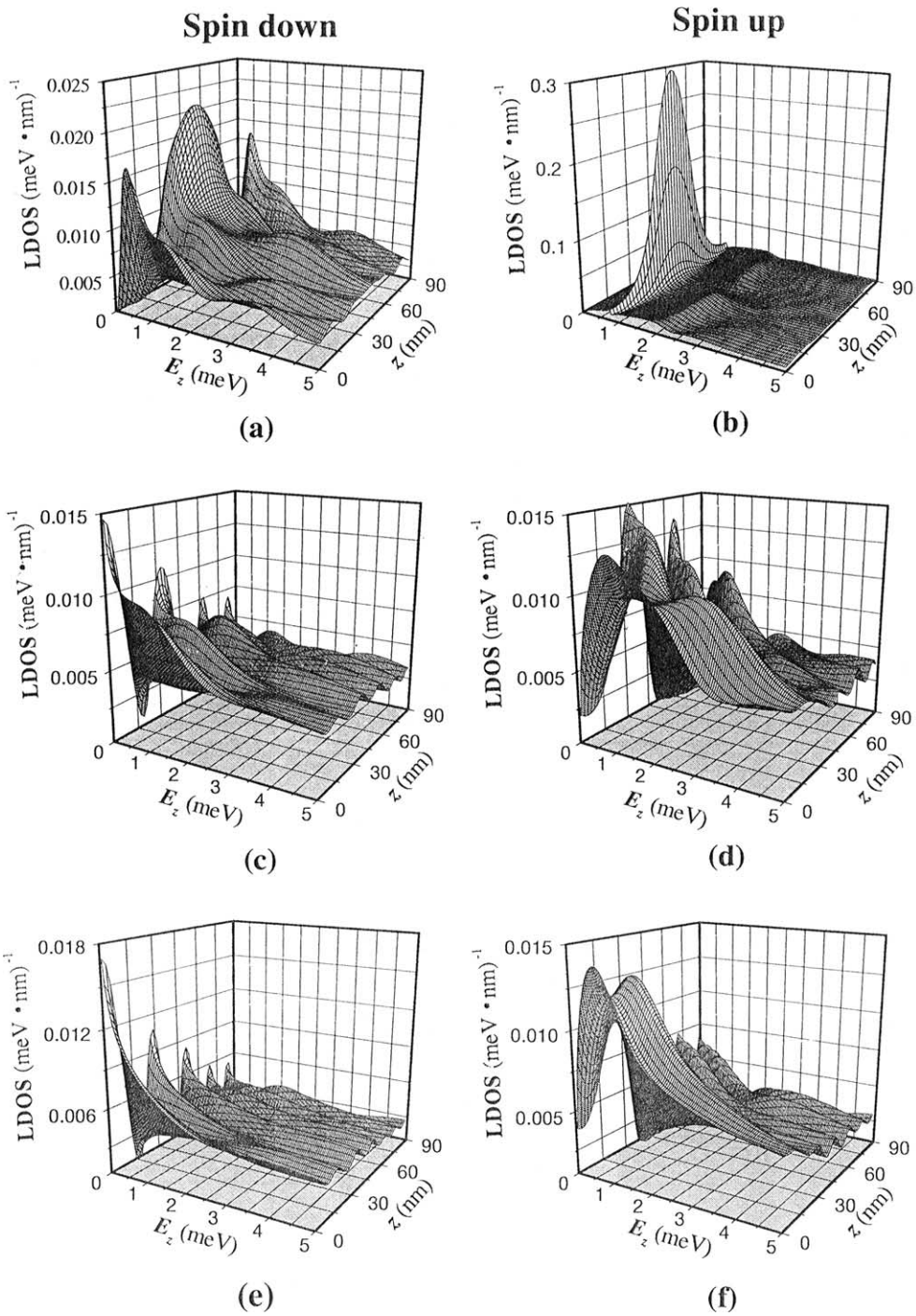

Fig. 3. LDOS distribution within $ZnSe/Zn_{1-x}Mn_xSe$ multilayers at zero bias and at applied biases. $L_0 = 30$ nm, $B = 0.5$ T. (a) and (b) $V_a = 0$ mV; (c) and (d) $V_a = 5$ mV; (e) and (f) $V_a = 10$ mV.

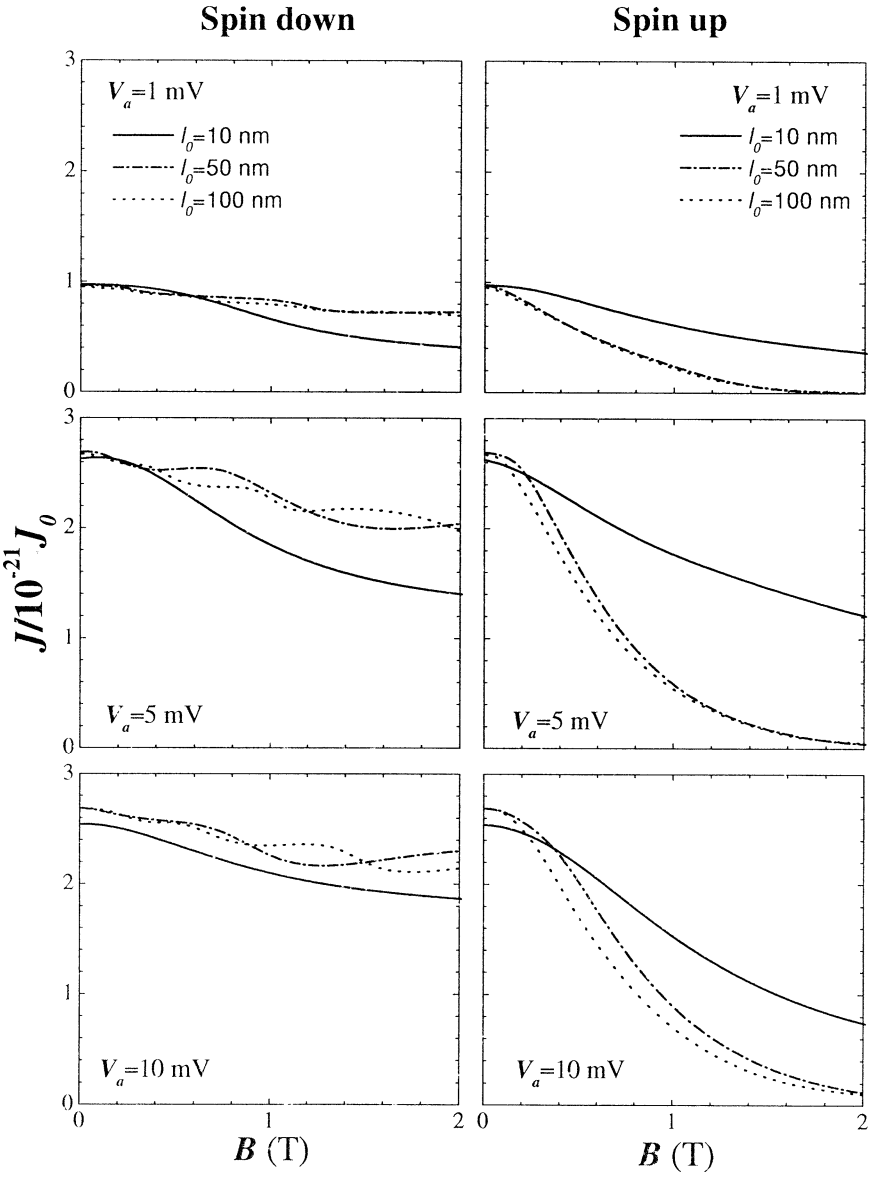

Fig. 4. Spin-dependent current densities for spin-up and spin-down electrons traversing $ZnSe/Zn_{1-x}Mn_xSe$ multilayers with different widths $L_0 = 10$, 50, 100 nm under several applied biases. $V_a = 1$, 5, 10 mV, $E_f = 5$ meV.

focus on the well region. Further, the LDOS distributions exhibit oscillations within the structure, which have the same intensity in both wells for spin down electrons as well as in both barriers for spin up electrons, i.e., the LDOS displays symmetric distributions with the center of the structure. The systems with different sizes also exhibit quite different spatial distributions of states. Under an applied bias, the corresponding spatial LDOS distributions over the multilayer differ essentially from those for zero bias case. The symmetry of the LDOS distributions is broken up. The oscillations become more complex and more rapid for

the larger size system. One can see the two systems with different sizes display quite different spatial distributions of the states, which results in the different resonance characteristics exhibited in the transmission spectra (see Fig. 1).

Now we examine to what extent spin polarization exhibited in spin-dependent current density. Fig. 4 shows the current density as the function of the magnetic field under several fixed biases $V_a = 1, 5, 10$ mV. One can see that the spin-down component of the current density decreases slowly as the magnetic field is increased, and displays oscillations for larger L_0 case. This behavior is a direct consequence of the resonance in $T_\downarrow(E_z, V_a, B)$. The spin-up current density is essentially exponentially decaying. This reflects the dominant exponentially suppression of $T_\uparrow(E_z, V_a, B)$ for increasing magnetic fields. Further, one can also see obvious quantum size effect on spin-dependent current density. As the size of the structure is increasing, the difference between the spin-down current density and spin-up current density is enlarged, which can be described by the spin polarization. The percentage polarization of the current can be defined as

$$P(B, V_a) = \frac{J_\uparrow(B, V_a) - J_\downarrow(B, V_a)}{J_\uparrow(B, V_a) + J_\downarrow(B, V_a)},$$

where $J_\uparrow$ and $J_\downarrow$ are the current density for spin-up and spin-down electrons, respectively. Here we do not present numerical results. However, in Fig. 4 one can easily see features of the spin polarization for electrons tunneling through $ZnSe/Zn_{1-x}Mn_xSe$ multilayers. At small applied magnetic fields, the degree of polarization is very small. As the magnetic field is increased, the degree of the polarization is raised. The thicker is the layers, the degree of polarization is higher. Moreover, for the system of a larger size, the degree of polarization is lowered with increasing the external electric field.

Finally, we examine to what extent the temperature affect on spin polarization for electrons tunneling through tunable $ZnSe/Zn_{1-x}Mn_xSe$ multilayers. In Ref. [17], the author made a first approximation investigations: the zero-bias and low-temperature transmission coefficient is adopted to calculate zero-temperature current density. In this work, we consider the influence of the finite temperature on both the transmission coefficient and the current density. In Fig. 5 we present the numerical comparison of the current densities between $T = 0$ K case and $T = 4.2$ K case. Although the difference between two considered temperatures is small, the discrepancy of the current densities is large. With increasing the temperature, the current density for both spin-down component and spin-up component are greatly enlarged. However, the degree of the spin polarization is drastically lowered with increasing the temperature. From Fig. 5, we see that the temperature greatly restricts spin-polarized transport. At zero temperature, one can obtain high degree of spin polarization electron beams. As the temperature is increasing, the degree of spin polarization will be drastically reduced.

4. Conclusions

In summary, we present tight-binding Green's function investigations of the influence of quantum sizes and the temperature on spin tunneling transport in $ZnSe/Zn_{1-x}Mn_xSe$ multilayers. It is confirmed that quantum sizes of the structure can play significant role in spin-polarized transport through the system. Not only spin-dependent transmission characteristics but also the degree of electron polarization can be greatly induced by the size of the corresponding structure. Numerical results indicate that the larger is the size of the corresponding structure, the higher the degree of electron polarization is. The effects of the external magnetic field and of the electric field on spin-polarized transport are also examined. The results show that as the magnetic field is increased, the degree of electron polarization is raised. It is further confirmed that the external electric field can greatly change the status of electron polarization. The spin-dependent tunneling features are reasonably illustrated by using the "concept" if the local density of states. Moreover, we also find that the degree of electron polarization is greatly lowered as the temperature is increasing.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (grant No. 10004006) and by the National Key Project of Basic Research Development Plan (grant No. 2000067107). Three of us (Y.G., J.-Q.L., and B.-L.G.) gratefully acknowledge

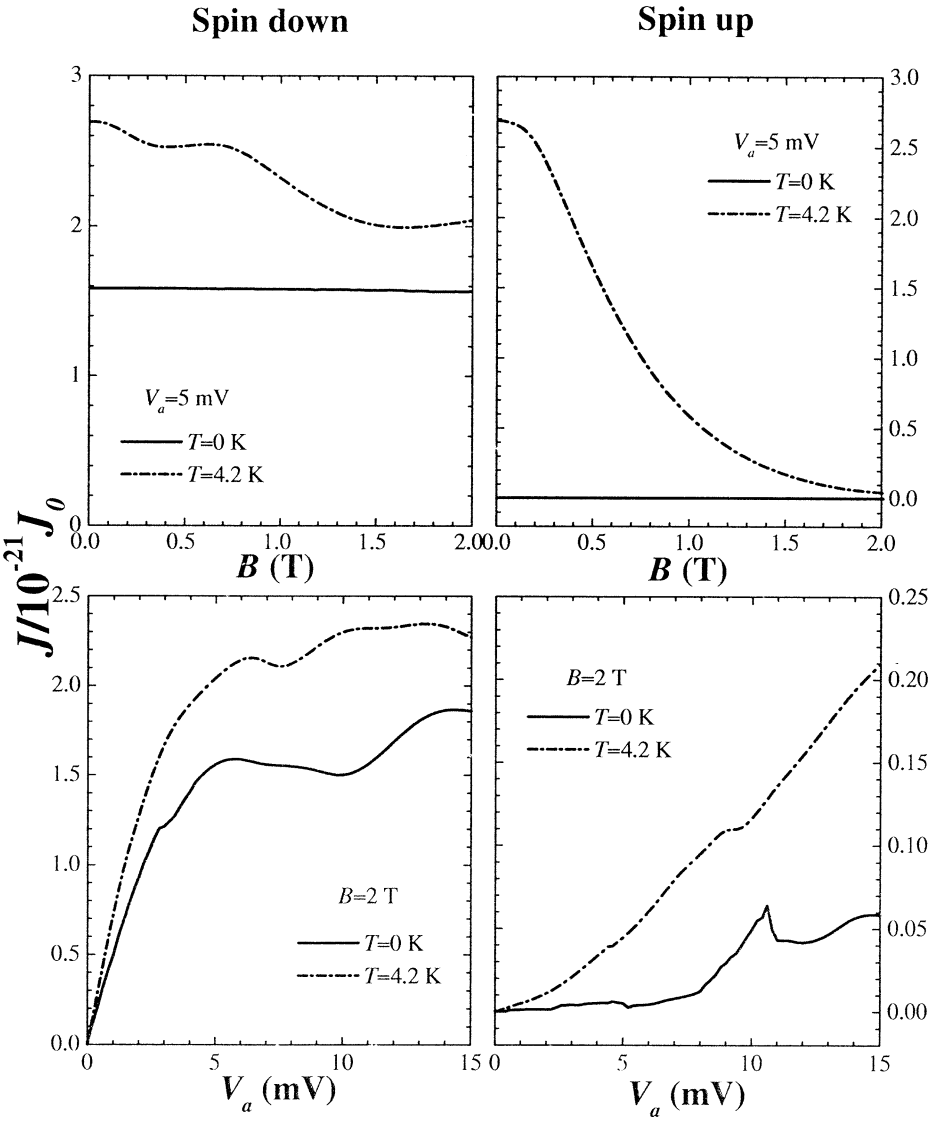

Fig. 5. Temperature dependence of current densities for spin-up and spin-down electrons traversing ZnSe/$Zn_{1-x}Mn_xSe$ multilayers. $L_0 = 50$ nm, $E_f = 5$ meV.

the cooperation with the Institute for Materials Research, Tohoku University, Japan.

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