Enhancement of the electronic effective mass in quantum wires

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(Received 22 February 1994)

We show that the nonparabolicity and spin splitting enhance electron effective mass appreciably in a quantum wire. In bulk materials, these effects are usually small since electrons are near the conduction-band edges. In quantum wires, strong confinement puts the electrons far from the conduction-band edge, giving rise to large nonparabolicity effects. We derive a simple expression for the effective mass parallel to the transport direction in the quantum wire, taking into account the band nonparabolicity, anisotropy, and spin splitting. We apply our formalism to $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wires and find that the parallel mass could be 50% more than the bulk value for a wire width of 50 Å.

I. INTRODUCTION

Low-dimensional semiconductor structures such as quantum wells and quantum wires have received great attention due to their electronic properties.[1–14] In these structures, the quantum confinement results in high mobility and suppressed scattering for the carriers.[9,14] This promises high-speed device applications.

The quantum confinement has profound influence also on the effective-mass approximation that is so commonly employed in modeling the quantum well and quantum wire structures. In a typical quantum well of 100 Å width, for example, the subband energy due to the well potential is approximately 50 meV in a $GaAs/Al_{0.3}Ga_{0.7}As$ structure. So the electronic motion is not usually near the bottom of the conduction band, contrary to the case in the bulk. Therefore the anisotropy and the nonparabolicity of the band structure have an unusually large effect on the effective mass than in the bulk material. Such an effect would result in a substantial increase in the electronic effective mass.[1–8] A proper treatment of this effect in the quantum wells has been given by Ekenberg.[8]

In this paper, we discuss the combined effects of the quantum confinement, band nonparabolicity, and spin splitting on the electron effective mass in quantum wires. We derive a simple expression for the effective mass that can be readily applied to practical structures. Compared with the case in the quantum wells, the wire structure has even stronger confinement. Therefore one expects that the effect of nonparabolicity will be much more pronounced in the quantum wires. We show that the electron effective mass is significantly enhanced compared to its bulk value. In most of the discussions about the transport properties of the quantum wires, the bulk effective mass is commonly used. This results in an overestimation of the carrier mobility.

The paper is arranged as follows. In Sec. II, we give the theory of the effect of band nonparabolicity on the electron effective mass in quantum wires. We follow an approach similar to that used by Ekenberg[8] in the case of quantum wells. In Sec. III, numerical results are presented for $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wires as an example. The parallel effective mass, which is relevant in the transport measurements in the quantum wire structures, is given as a function of the wire thickness. For a wire thickness of 50 Å, the electronic effective mass is almost 50% enhanced over the bulk value.

II. THEORETICAL TREATMENT

We begin with the conduction-band dispersion in bulk GaAs. According to the $\mathbf{k}\cdot\mathbf{p}$ theory, the structure of the conduction band can be specified by the expression[15]

$$E(\mathbf{k})=\frac{\hbar^2k^2}{2m_1}+\alpha_0k^4+\beta_0(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2) \pm\gamma_0[k^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)-9k_x^2k_y^2k_z^2]^{1/2} \quad (1)$$

expanded up to fourth order in $\mathbf{k}$. The parameters appearing in Eq. (1) are as follows: $m_1=0.067m_0$ is the effective mass of the electron in bulk GaAs, m_0 being the free electron mass, $\alpha_0=-1.969\times10^{-29}$ eV cm^4, $\beta_0=-2.306\times10^{-29}$ eV cm^4, and $\gamma_0=-2.8\times10^{-23}$ eV cm^3. The term proportional to β_0 describes the conduction-band anisotropy while the last term gives the spin splitting which is due to the broken inversion symmetry in GaAs.

We assume that the quantum wire has a square cross section and is along the z direction. Since there is translation invariance along z, k_z remains a good quantum number. The subband levels due to the confinement in the x-y direction can be determined by setting $k_z=0$ first and replacing k_x and k_y by $-\partial/\partial x$ and $-\partial/\partial y$ in (1). The equation of motion therefore becomes

$$\left[-\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\beta_0\left(\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2}\right) +\alpha_0k^4\pm\gamma_0\sqrt{k^2(k_x^2k_y^2)}\right]\psi=E(\mathbf{k})\psi . \quad (2)$$

It can easily be verified that the solutions of the Schrödinger equations in the nonparabolic case are of the form $\cos(k_xx)\cos(k_yy)$ (in the well) and $\exp(-\lambda x)\exp(-\lambda y)$ (in the barrier) where

$$\lambda=\sqrt{2m_2(V_0-\varepsilon)/\hbar^2}\ , \tag{3}$$

and the energy ε is given by

$$\varepsilon=-\frac{\hbar^2}{2m_1}(k_x^2+k_y^2)+\beta_0(k_x^2k_y^2)+\alpha_0k^4 \pm\gamma_0\sqrt{k^2(k_x^2k_y^2)}\ , \tag{4}$$

where V_0 is the conduction-band discontinuity between GaAs and $Al_{0.3}Ga_{0.7}As$ and m_2 is the effective mass in $Al_{0.3}Ga_{0.7}As$. In solving for the subband energy ε, we use the boundary conditions with continuity of the envelope function and its derivative divided by the effective mass in the bulk. This leads to the following coupled nonlinear equations for k_x and k_y for the lowest subband:

$$\tan(k_xL/2)=\frac{m_1}{m_2}\frac{\lambda}{k_x} \tag{5a}$$

and

$$\tan(k_yL/2)=\frac{m_1}{m_2}\frac{\lambda}{k_y}\ , \tag{5b}$$

where L is the width of the quantum wire.

To obtain the expression for the effective mass of the electron in the z direction, we go back to Eq. (1) and isolate the terms containing k_z^2 as follows:

$$E(\mathbf{k})=\frac{\hbar^2}{2m_1}k_z^2+(2\alpha_0+\beta_0)(k_x^2+k_y^2)k_z^2 \pm\gamma_0\{(k_x^2+k_y^2)(k_x^2k_y^2) +[(k_x^2+k_y^2)^2-8k_x^2k_y^2]k_z^2\}^{1/2}+O(k_z^4)\ . \tag{6}$$

First, we neglect spin splitting. We have from Eq. (6) then

$$E(\mathbf{k})=\left[\frac{\hbar^2}{2m_1}+(2\alpha_0+\beta_0)(k_x^2+k_y^2)\right]k_z^2\ . \tag{7}$$

Setting the above expression to be equal to $\hbar^2k_z^2/2m_\parallel^*$, we obtain the effective mass after the nonparabolicity correction as

$$m_\parallel^*=\frac{m_1}{[1-(2\alpha+\beta)(\hbar^2/2m_1)(k_x^2+k_y^2)]}\ , \tag{8}$$

where we have defined

$$\alpha=-(2m_1/\hbar^2)^2\alpha_0 \tag{9a}$$

and

$$\beta=-(2m_1/\hbar^2)^2\beta_0\ . \tag{9b}$$

With spin splitting included we define

$$A=(k_x^2+k_y^2)(k_x^2k_y^2)\ , \tag{10a}$$

$$B=(k_x^2+k_y^2)^2-8k_x^2k_y^2\ , \tag{10b}$$

and

$$C=(k_x^2+k_y^2)\ , \tag{10c}$$

then the last term in Eq. (1) can be rewritten as

$$\begin{aligned}&\pm\gamma_0\{(k_x^2+k_y^2)(k_x^2k_y^2)+[(k_x^2+k_y^2)^2-8k_x^2k_y^2]k_z^2+(k_x^2+k_y^2)k_z^4\}^{1/2}\\ &=\pm\gamma_0A^{1/2}\sqrt{1+(1/A)(B+Ck_z^2)k_z^2}\\ &=\pm\gamma_0A^{1/2}\left[1+\frac{1}{2}\frac{1}{A}(B+Ck_z^2)k_z^2-\frac{1}{8}\frac{1}{A^2}(B+Ck_z^2)^2k_z^4+O(k_z^6)\right]\\ &=\text{const}\pm\frac{1}{2}\gamma_0\frac{B}{A^{1/2}}k_z^2+O(k_z^4)\ .\end{aligned} \tag{11}$$

Combined with the rest of the terms in Eq. (6), we have

$$E(\mathbf{k})=\left[\frac{\hbar^2}{2m_1}+(2\alpha_0+\beta_0)(k_x^2+k_y^2)\pm\frac{\gamma_0}{2}\frac{B}{\sqrt{A}}\right]k_z^2=\frac{\hbar^2}{2m_\parallel^*}k_z^2\ . \tag{12}$$

Therefore after taking into account the spin splitting, the effective mass is given by

$$m_\parallel^*=\frac{m_1}{\left[1-(2\alpha+\beta)\left[\frac{\hbar^2}{2m_1}\right](k_x^2+k_y^2)\pm\frac{\gamma}{2}\left[\frac{\hbar^2}{2m_1}\right]^{1/2}\frac{B}{\sqrt{A}}\right]}\ , \tag{13}$$

where

$$\gamma=-\gamma_0\left[\frac{2m_1}{\hbar^2}\right]^{3/2}\ . \tag{14}$$

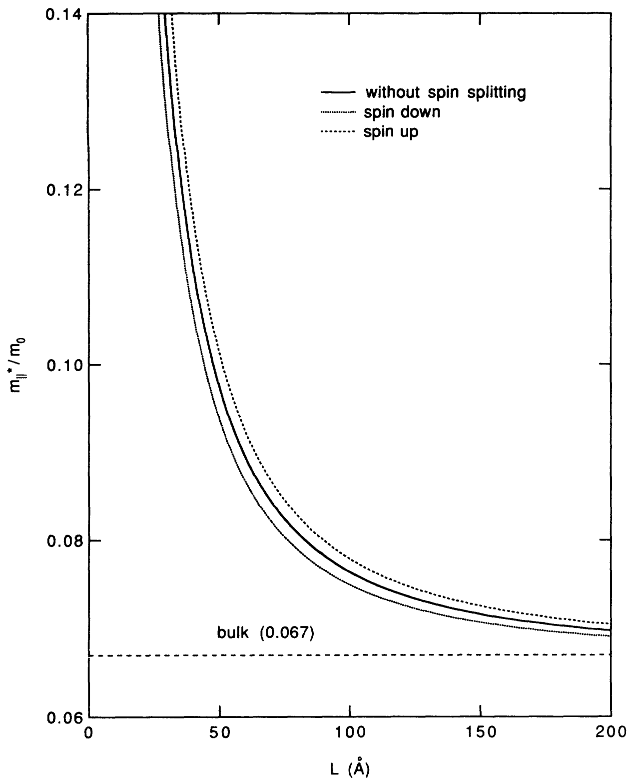

FIG. 1. Variation of the electron effective mass in the parallel direction ($m_{\parallel}^*$) expressed in terms of free electron mass (m_0) as a function of the wire width.

In Eqs. (8) and (13), the dependence of the effective mass $m_{\parallel}^*$ on the wire width L and the conduction-band offset V_0 comes through terms which depend on k_x and k_y. The explicit dependence of $m_{\parallel}^*$ on L and V_0 is determined by solving for k_x and k_y from Eqs. (5a) and (5b) and substituting their values in Eqs. (8) and (13).

III. RESULTS AND DISCUSSIONS

We consider quantum wires of $GaAs/Al_{0.3}Ga_{0.7}As$, taking the conduction-band discontinuity to be 247 meV and use $m_2 = 0.099m_0$ for the mass in the barrier.[16] In Fig. 1, we show the wire width dependence of the effective mass with and without spin splitting. The effective mass increases monotonically with decreasing thickness. The spin splitting does not alter the results significantly. Generally there is a large enhancement of the effective mass for wire width below 100 Å. At 50 Å the effective mass is almost 50% more than the bulk value.

The increase in the effective mass of the electron will affect physical properties such as mobility in the quantum wires directly. Recent experiments on electron transport in $GaAs/Al_xGa_{1-x}As$ quantum wires show that carrier mobilities vary considerably for different wire dimensions.[17–19] Given the current status of the quality of the wire structures, it is hard to discern the true effect of the confinement from that of defects and additional scattering caused by wire-width fluctuations. So a direct verification of the enhancement of the carrier effective mass in these structures is not available yet.

It should be noted that the penetration of the electronic wave function into the barrier region leads to additional complications in the determination of the carrier mobility from the effect studied in this paper alone. In $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wires of width 2 nm, for example, almost 50% of the wave function would be in the barrier region. Since bulk $Al_{0.3}Ga_{0.7}As$ has a larger electron effective mass than the well material GaAs, the overall effect is to increase the electronic effective mass, and thus lower the mobility. This barrier penetration effect has not been taken into account in our discussion. However it can be estimated that this effect will be significant below wire width of approximately 2 nm. Therefore for wire widths below that range, the results obtained here will not be expected to be very accurate.

In conclusion, we have studied the effects of nonparabolicity and spin splitting on the electron effective mass in the parallel direction of the quantum wires. The parallel effective mass, which is of importance for transport properties in the quantum wires, is shown to be significantly enhanced compared to the bulk value in GaAs. We have derived a simple expression for the parallel effective mass which can be easily applied to practical structures. For $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wire structures, the parallel effective mass is given as a function of the well width and is shown to be at least 50% enhanced over the bulk value at wire width of 50 Å.

ACKNOWLEDGMENTS

This work was supported by the Air Force Office of Scientific Research under Grant No. AFOSR-91-0056.

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