MODIFICATION OF THE THEORY OF ONE-DIMENSIONAL MOBILITY DUE TO SCATTERING BY A DISORDERED ALLOY

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UDC 539

Analytic expressions are derived for the electron mobility and relaxation rate in a rectangular quantum wire for the scattering by a disordered alloy. The dependence of the electron mobility on temperature and a transverse dimension is numerically evaluated. It is found that the mobility increases continuously, because no new intersubband scattering contributes. It is shown that the alternate increase and decrease of the mobility depending on the transverse dimension of a quantum wire occur due to intersubband scattering.

Introduction

Recently, there has been a considerable interest in systems in which the electron motion is confined to one or two dimensions. The most interesting situation occurs when the confinement is of the order of the de Broglie wavelength for electrons. In a quantum wire, when its width becomes much less than the mean free path, the motion of electrons becomes quasi-one-dimensional (Q1D). The motion of electrons in such semiconductor structures leads to size quantization effects [1—10]. The physical properties of low-dimensional semiconductor structures differ from those of bulk semiconductors, because the translational symmetry is broken [11]. The study of electron transport properties of a Q1D electron gas in semiconductor structures has continued to be a subject of academic interest from the viewpoint of the design of devices. The mobility of electrons in rectangular [1—2] and cylindrical [3—8] quantum wires (QW) has been investigated theoretically for many different scattering mechanisms. There have been calculations of the electron scattering by acoustic phonons [1], the impurity-limited mobility [4, 8], phonon-limited mobility [3], and the mobility of electrons scattered by impurities and by acoustic and polar optical phonons [2, 9]. The alloy-disorder-induced scattering is an important scattering mechanism when a confining quantum well consists of a ternary semiconductor. The alloy-disorder-induced scattering in ternary compound semiconductors and quantum-well structures has been the subject of many theoretical and experimental investigations [12—29]. Recently [7], the electron mobility and electron scattering by disordered alloys have been studied theoretically for cylindrical quantum-well wires. In works [1—9], the electron mobility was evaluated in the size quantum limit, and intersubband scattering was neglected.

The present work deals with both the derivation of expressions for the momentum relaxation time associated with the "electron — alloy-disorder" interactions and the calculation of the mobility of the Q1D electron gas in rectangular quantum wires. We also consider the effect of intersubband scattering on the mobility.

1. Formalism

We consider a QW made of an alloy denoted by the symbol $A_{1-x}B_xC$. We assume that a gas of carriers is confined to move in a long thin wire that is embedded in an insulating cladding. For simplicity, we choose the cross section of the wire to be rectangular with the cross sectional dimensions a and b along the x and y directions, respectively, and with the wire length L along the z direction where electrons are assumed to move freely. Assuming the usual effective-mass approximation for the conduction band , the energy eigenfunctions and eigenvalues for electrons in a rectangular thin wire can be written as

$$E_{knl} = E_k + E_n + E_l = \frac{\hbar^2 k^2}{2m} + n^2 E_a^0 + l^2 E_b^0,$$

$$E_a^0 = \frac{\pi^2\hbar^2}{2m^* a^2}, \quad E_b^0 = \frac{\pi^2\hbar^2}{2m^* b^2}, \quad n, l = 1, 2, 3, \ldots, \qquad (1)$$

$$\Psi_{knl} = [2/(abL)^{1/2}] \sin(\pi n x/a) \sin(\pi l y/b) \exp(ikz).$$

When the confining quantum well consists of a ternary semiconductor (like $Ga_{1-x}In_xAs$), in the virtual

crystal approximation, the alloy-disorder scattering potential is as follows [19—22]:

$$H_{\rm dis} = \delta V \Big\{ (1-x) \sum_{r_{\rm In}} Y_{\Omega_0}(r - r_{\rm In}) -$$

$$- x \sum_{r_{\rm Ga}} Y_{\Omega_0}(r - r_{\rm Ga}) \Big\}, \qquad (2)$$

where $Y_{\Omega_0}(r_a - r_b) = 1$ when r_a and r_b are inside the same unit cell and vanish elsewhere, the summations run over all the unit cells, and Ω_0 is the volume of the unit cell.

The momentum relaxation time τ of electrons in a Q1D system due to the scattering potential $H_{\rm dis}$ is given by the relaxation rate [30]

$$\tau^{-1} = \frac{2\pi}{\hbar} \sum_f |\langle f|H_{\rm dis}|i\rangle|^2 (1 - \cos\theta) \delta(E_f - E_i). \qquad (3)$$

Here, i and f represent the initial and final states and θ is the angle between the incident and scattered wave vectors of electrons along the axis of the wire.

Using this form of the potential, the square matrix element for the transition from a state knl to another state $k'n'l'$ may be expressed as [17]

$$|\langle k'n'l'|H_{\rm dis}|knl\rangle|^2 = \frac{\Omega_0}{V} (\delta V)^2 x(1-x) \times$$

$$\times \left(1 + \frac{1}{2}\delta_{nn'}\right) \left(1 + \frac{1}{2}\delta_{ll'}\right). \qquad (4)$$

Substituting Eq.(4) in Eq.(3), we find that the momentum relaxation rate for electron—alloy-disorder scattering is given by

$$\frac{1}{\tau_{\rm alloy}} = \frac{\sqrt{2}\Omega_0 (\delta V)^2 x(1-x) m^{*1/2}}{ab\hbar^2} \times$$

$$\times \sum_{n'l'} \frac{\left(1 + \frac{1}{2}\delta_{nn'}\right)\left(1 + \frac{1}{2}\delta_{ll'}\right)}{\left[E_{nlk} - E_{n'} - E_{l'}\right]^{1/2}}. \qquad (5)$$

For comparison, we also give the result obtained for the momentum relaxation rate of electron-acoustic phonon scattering in a Q1D system [2]:

$$\frac{1}{\tau_{\rm ac}} = \frac{2\sqrt{2}E_d^2 k_{\rm B} T m^{*1/2}}{ab\hbar^2 \rho v_s^2} \sum_{n'l'} \frac{\left(1 + \frac{1}{2}\delta_{nn'}\right)\left(1 + \frac{1}{2}\delta_{ll'}\right)}{\left[E_{nlk} - E_{n'} - E_{l'}\right]^{1/2}}.$$

The identical nature of variation for the two scattering processes may be explained by examining the matrix elements for scattering. The ratio $\tau_{\rm alloy}^{-1}/\tau_{\rm ac}^{-1}$ is

$$\frac{\tau_{\rm alloy}^{-1}}{\tau_{\rm ac}^{-1}} = \frac{(\delta V)^2 \Omega_0 x(1-x)\rho v_s^2}{2E_d^2 k_{\rm B} T}.$$

For $Ga_{0.8}In_{0.2}As$, we find $\tau_{\rm alloy}^{-1}/\tau_{\rm ac}^{-1} = 420/T$, so that momentum relaxation rate for electron — alloy-disorder scattering is higher than that for electron — acoustic phonon scattering.

It is interesting to note that, in the quantum size limit, we can assume $n = n\prime = l = l\prime = 1$ in the temperature range where the intersubband transitions are not allowed due to energy differences between the subbands being very large (i.e. $E_a^0/k_{\rm B}T > 1$, $E_b^0/k_{\rm B}T > 1$). In this case, the expression for $\tau_{\rm alloy}^{-1}$ is reduced to

$$\frac{1}{\tau_{\rm alloy}} = \frac{9\Omega_0 (\delta V)^2 x(1-x) m^{*1/2}}{2\sqrt{2E_k} ab\hbar^2}. \qquad (6)$$

For the intrasubband scattering, Eq.(6) yields that the scattering rate increases and the momentum relaxation time decreases as the transverse dimension of the wire decreases for the scattering by alloy-disorder. A formula similar to Eq.(6) has been obtained by Ando [20] and Bastard [21] for a Q2D electron gas.

When it is feasible to define a momentum relaxation time, the mobility μ can be written as

$$\mu = \frac{e}{m^*} \langle \tau \rangle, \qquad (7)$$

where $\langle ... \rangle$ means the average defined by the expression

$$\langle ... \rangle = \frac{\sqrt{2} m^{*1/2}}{\pi\hbar n_{1D}} \sum_{nl} \int E_k^{1/2} (...) \frac{\partial f_0(E_{knl})}{\partial E_{knl}} dE_k, \qquad (8)$$

where $f_0(E_{knl})$ is the distribution function for the carriers in the wire and n_{1D} is the density of electrons per unit length of the wire.

For the case of a nondegenerate Q1D electron gas, the electron distribution function is

$$f_0(E_{knl}) = \frac{(2\pi)^{1/2} \hbar n_e ab}{\gamma\delta (m^* K_{\rm B} T)^{1/2}} \exp\left[-\frac{n^2 E_n^0 + l^2 E_l^0}{K_{\rm B} T} \right] \times$$

$$\times \exp\left(-\frac{E_K}{K_{\rm B} T} \right), \qquad (9)$$

where $\gamma = \sum_n \exp\left(-\frac{n^2 E_n^0}{K_{\rm B}T}\right)$, $\delta = \sum_l \exp\left(-\frac{n^2 E_l^0}{K_{\rm B}T}\right)$ and n_e is the concentration of electrons. From this expression, the Fermi energy can be identified as

$$\xi = K_{\rm B} T \ln\left(\frac{\sqrt{2\pi}\hbar n_{1D}}{\gamma\delta (m^* K_{\rm B} T)^{1/2}} \right). \qquad (10)$$

For the case of a nondegenerate carrier statistics, the mobility is given by

$$\mu_{\rm alloy}^{1D} = \frac{4eab\hbar^2}{\sqrt{2\pi}m^{*3/2}\Omega_0\left(\delta V\right)^2 x\left(1-x\right) Z\gamma\delta\left(K_{\rm B}T\right)^{3/2}}\times$$

$$\times\sum_{nl}\exp\left(-\frac{E_{nl}}{K_{\rm B}T}\right)\left[-B_{nn'll'}^2\exp\left(\frac{B_{nn'll'}}{K_{\rm B}T}\right)\times\right.$$

$$\left.{\rm E}i\left(-\frac{B_{nn'll'}}{K_{\rm B}T}\right) - B_{nn'll'}K_{\rm B}T + \left(K_{\rm B}T\right)^2\right], \qquad (11)$$

where

$$Z = 2\left(n'l'\right) + n' + l' + \frac{1}{2},$$

$$B_{nn'll'} = \left[\sum_{n'l'}\left(E_{n'} + E_{l'} - E_n - E_l\right) + \right.$$

$$\left. + \frac{1}{2}\sum_{n'}\left(E_{n'} - E_n\right) + \frac{1}{2}\sum_{l'}\left(E_{l'} - E_l\right)\right]/Z. \qquad (12)$$

Here, ${\rm E}i\left(-x\right) = \int\limits_{-\infty}^{-x}\frac{e^t}{t}dt$ is the integrated indicative function.

When the carriers are degenerate, $f_0(E_{knl})$ is given at low temperatures by the Fermi-Dirac distribution and the mobility is ${\rm e}\tau(\xi)/{\rm m}^*$:

$$\mu_{\rm alloy}^{1D} = \frac{2eab\hbar^2}{\pi n_{1D}m^*\Omega_0\left(\delta V\right)^2 x\left(1-x\right) Z}\times$$

$$\times\sum_{nl}\frac{\left[\xi - \left(E_n + E_l\right)\right]^2}{\left[\xi - \left(E_n + E_l\right) + B_{nn'll'}\right]}, \qquad (13)$$

where the Fermi energy ξ in this degenerate limit can be shown, in the standard way, to be given by

$$n_{1D} = \frac{\left(2m^*K_{\rm B}T\right)^{1/2}}{\pi\hbar}\sum_{nl}F_{1/2}\left(\frac{\xi - \left[E_n + E_l\right]}{K_{\rm B}T}\right). \qquad (14)$$

Here, $F_1(\eta)$ is the well-known Fermi integral [30].

In the size quantum limit, in the general case, there are no approximations for $f_0(E_{knl})$. From Eqs. (6)—(8), the mobility can be written as

$$\mu_{\rm alloy}^{1D} = \frac{4eab\hbar K_{\rm B}TF_1\left(\frac{\xi - 2E_a^0}{K_{\rm B}T}\right)}{9\Omega_0\pi m^*n_{1D}\left(\delta V\right)^2 x\left(1-x\right)}. \qquad (15)$$

It can be seen that, in Eq. (15) in the intrasubband scattering case, the mobility increases with the transverse dimensions of the wire. In the size quantum limit, Eq. (11) is written as

$$\mu_{\rm alloy}^{1D} = \frac{4\sqrt{2K_{\rm B}T}eab\hbar^2}{9\sqrt{\pi}m^{*3/2}\Omega_0\left(\delta V\right)^2 x\left(1-x\right)}. \qquad (16)$$

It is worth noting that the mobility due to alloy-disorder scattering in 3- and 2-dimensional systems has a functional dependence on temperature according to $T^{-1/2}$ [11] and T^0 [14, 21], respectively.

Eqs. (13)—(16) show that the μ varies as T^0 at low temperatures and as $T^{1/2}$ at high temperatures. This occurs because the density of states in 3-, 2-, and 1-dimensional systems has a functional dependence on energy according to $E^{1/2}$, E^0, and $E^{-1/2}$, respectively.

If μ_2 is the alloy-scattering mobility in a Q2D system [23], then a nondegenerate electron distribution is

$$\frac{\mu_{\rm alloy}^{1D}}{\mu_{\rm alloy}^{2D}} = \frac{3\pi^{3/2}ab\left(K_bTm^*\right)^{1/2}}{16\sqrt{2}d\hbar}, \qquad (17)$$

where d is the thickness of the well.

On the other hand, for a completely degenerate electron distribution in the size quantum limit, we have

$$\frac{\mu_{\rm alloy}^{1D}}{\mu_{\rm alloy}^{2D}} = \frac{27\pi^2abm^{*1/2}\left(\xi - 2E_a^0\right)}{16d\hbar}. \qquad (18)$$

It can be seen from Eqs. (17)—(18) that the ratio of electron mobility in a Q1D system to that in a Q2D system depends not only on temperature but also on the size of the cross section of a quantum wire.

2. Numerical Analysis and Discussion

We have obtained the general expressions for the momentum relaxation rate and electron mobility in a rectangular quantum wire for scattering due to alloy disorder. Electron mobility is expressed as a function of transverse dimensions of the wire and temperature. On the basis of the obtained expressions, we have drawn Figs. 1—3. As a numerical example, we consider the electron mobility in a $Ga_{0.47}In_{0.53}As$ quantum wire for the alloy-disorder scattering. Relevant values of the physical parameters are taken to be $\delta V = 0.6$ eV, $m^*(Ga_{0.47}In_{0.53}As)=0.04m_0$, $\Omega_0 = \frac{5.87^3A^0}{4}$.

Fig. 1 shows the temperature dependence of the mobility due to the alloy disorder scattering in the size quantum limit for various Q1D systems of selected transverse dimensions. For comparison, we also plot the total mobility due to acoustic phonons, polar optical phonons, and background impurity scattering for a

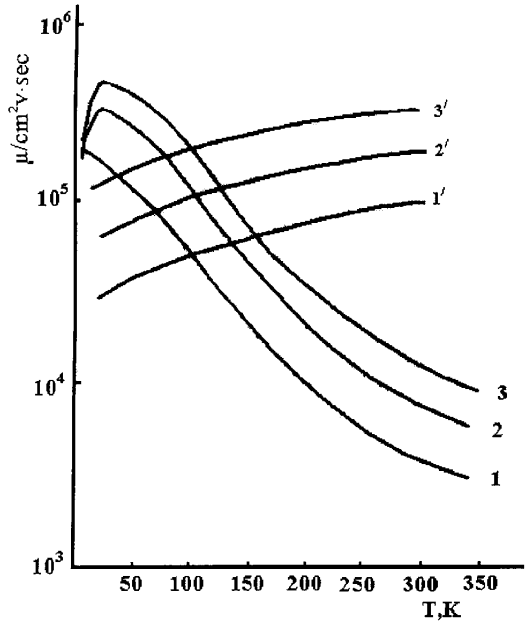

Fig. 1. Electron mobility for a Q1D structure for alloy-disorder scattering is plotted as a function of temperature with various values of transverse dimensions of a wire ($1'2'3'$). Curves *1*, *2*, and *3* correspond to the total electron mobility due to acoustic phonon, polar optical phonon, and background impurity scattering in Q1D systems [2]. We have chosen $a = 10$ nm ($1, 1'$), $a = 15$ nm ($2, 2'$), $a = 20$ nm ($3, 3'$)

GaAs rectangular quantum wire [2]. It is shown that the mobility considerably increases with the cross-sectional area of the wire. It was predicted in [17] that the free-carrier absorption coefficient due to alloy-disorder scattering in Q1D structures decreases with increase in transverse dimensions of the wire. This diminution in the free-carrier absorption coefficient explains the increase in the mobility predicted by our present results. As other scattering mechanisms (polar optical [2] and acoustic phonons [1, 2]), the mobility-limited alloy-disorder scattering also increases with increase in the cross-sectional area of the wire.

In Fig. 2, we show the electron mobility as a function of the transverse dimension of a wire at 300 K. It is shown that the alternate increase and decrease of the mobility depend on the transverse dimensions of a quantum wire. It is also shown that, because no new intersubband scattering contributes, the mobility increases with the transverse dimension of a wire. At 300 K, the electron distribution is classical, and electrons are thermally distributed over energy roughly up to about k_BT. Consequently, the appearance of the

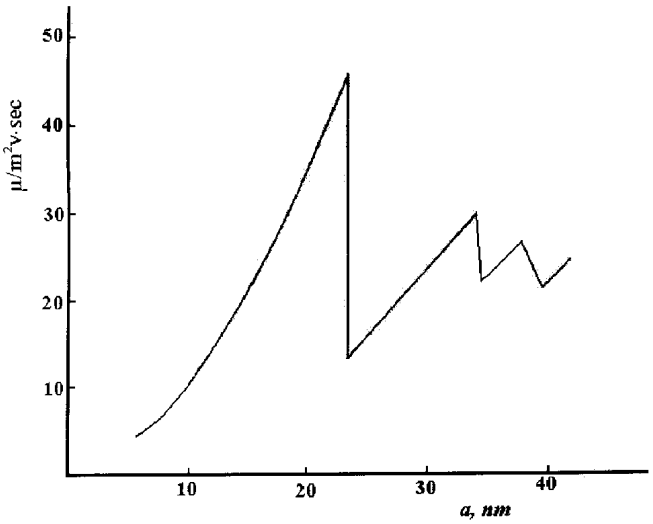

Fig. 2. Electron mobility as a function of the transverse dimension of a wire at 300 K

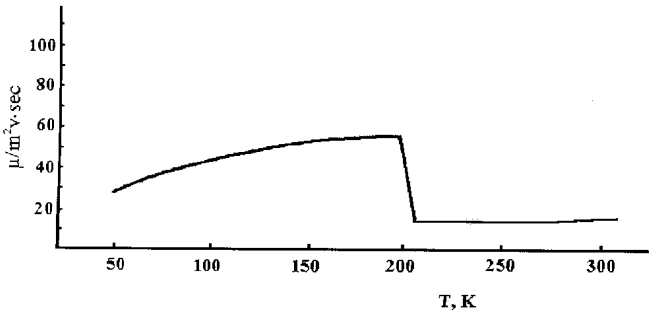

Fig. 3. Temperature dependence of the mobility due to alloy-disorder scattering at $a = b = 33$ nm

intersubband scattering due to alloy-disorder into the subband n is roughly determined by the condition

$$k_BT \geq E_{l1} \equiv E_l - E_1. \quad (19)$$

It is clear that the mobility peak corresponds roughly to the transverse dimensions where Eq.(19) is satisfied.

In Fig. 3, we show the temperature dependence of the electron mobility at $a = b = 33$ nm. Because no new intersubband scattering contributes, the mobility increases continuously for $T < 200$ K.

The author would like to thank M. I. Aliev, B. M. Askerov and F. M. Gashimzade for helpful discussions.

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Received 22.04.03

МОДИФІКАЦІЯ ТЕОРІЇ ОДНОВИМІРНОЇ РУХЛИВОСТІ, ЗУМОВЛЕНОЇ РОЗСІЯННЯМ НА НЕВПОРЯДКОВАНОМУ СПЛАВІ

Г.Б. Ібрагімов

Р е з ю м е

Отримано аналітичні вирази для часу релаксації і рухливості електронів провідності при розсіянні на невпорядкованостях сплаву у прямокутному напівпровідниковому квантовому дроті. Із залежності рухливості електронів від температури і поперечного перерізу дроту випливає, що, коли відсутнє міжпідзонне розсіяння, рухливість неперервно збільшується. Встановлено, що збільшення і зменшення рухливості електронів в залежності від поперечного перерізу квантових дротів зумовлено міжпідзонним розсіянням.