

# On Electron Mobility in a Rectangular Quantum Wire due to Alloy Disorder

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Received 22.09.2003

## Abstract

Analytic expressions are derived to describe the electron mobility and relaxation rate in the rectangular quantum wire experiencing scattering due to alloy disorder. The dependence of electron mobility on the temperature and transverse dimension is numerically evaluated and it is found that the mobility increases continuously with temperature, because there is no new intersubband scattering with increase in temperature. It is shown that the alternating increase/decrease in the mobility—depending on the transverse dimension of the quantum wire—occurs due to intersubband scattering. It is found that the mobility in a quantum wire is significantly greater than mobility in a quantum well.

## 1. Introduction

Recently there has been considerable interest in systems in which electron motion is confined to one or two dimensions. The most interesting situation occurs when the confinement is on the order of the de Broglie wavelength for confined electrons. In a quantum wire, when its width becomes much less than the mean free path, the motion of the electrons within becomes quasi-one-dimensional (Q1D). The motion of electrons in such semiconducting structures thus leads to size quantization effects [1–10]. The physical properties of low-dimensional semiconducting structures differ from the properties 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 a device point of view. The mobility of electrons in rectangular [1–2] and cylindrical [3–8] quantum wire has been investigated theoretically for many different scattering mechanisms. There have been modeling of electron scattering by acoustic phonons [1], impurity-limited mobility [4, 8], phonon-limited mobility [3], the mobility of electrons scattered by impurities, and by acoustic and polar optical phonons [2, 9]. Scattering due to alloy disorder is an important mechanism when the confining quantum well is a ternary semiconductor and has been subject of many theoretical and experimental investigations [12–28]. Electron mobility and electron scattering by alloy-disorder has been recently studied theoretically in cylindrical quantum well wires in [7]. In [1–9] electron mobility is evaluated in the size quantum limit, neglecting intersubband scattering.

In the present study, we deal with a derivation of expressions for the momentum relaxation time associated with electron-alloy disorder interactions, and calculation of the mobility of the Q1D electron gas in rectangular quantum wires. We also consider intersubband scattering effects on mobility.

## 2. Formalism

We consider the QW of a three part alloy, denoted symbolically as  $A_{1-x}B_xC$ . We assume that a gas of carriers is confined to move along a thin wire embedded in insulating cladding. For simplicity, we choose the cross section of the wire to be rectangular of cross-sectional dimensions  $a \cdot b$ , the dimensions along the  $x$  and  $y$  directions, respectively; with 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 follows:

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

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

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

When the confining quantum well consists of a ternary semiconductor (such as  $\text{Ga}_{1-x}\text{In}_x\text{As}$ ), in the virtual crystal approximation, the alloy-disorder scattering potential assumes the following form [19–22]:

$$H_{dis} = \delta V \left\{ (1-x) \sum_{r_{In}} Y_{\Omega_0}(r - r_{In}) - x \sum_{r_{Ga}} Y_{\Omega_0}(r - r_{Ga}) \right\}. \quad (2)$$

Here,  $Y_{\Omega_0}(r_a - r_b) = 1/\Omega_0$  when  $r_a$  and  $r_b$  are inside the same unit cell and vanishes elsewhere. The summations run over all the unit cells, and  $\Omega_0$  is the volume of the unit cell. The momentum relaxation time  $\tau$  of the electrons in a Q1D system due to the scattering potential  $H_{dis}$  is given by the relaxation rate [29] as

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

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

Using (3) for the form of the potential, the square matrix element for transition from state  $knl$  to state  $k'n'l'$  may be expressed as [17]

$$|\langle k'n'l' | H_{dis} | knl \rangle|^2 = \frac{\Omega_0}{V} (\delta V)^2 x(1-x) \left( 1 + \frac{1}{2} \delta_{nn'} \right) \left( 1 + \frac{1}{2} \delta_{ll'} \right). \quad (4)$$

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

$$\frac{1}{\tau_{alloy}} = \frac{\sqrt{2} \Omega_0 (\delta V)^2 x(1-x) m^{*1/2}}{ab \hbar^2} \sum_{n'l'} \frac{(1 + \frac{1}{2} \delta_{nn'}) (1 + \frac{1}{2} \delta_{ll'})}{[E_{nlk} - E_{n'} - E_{l'}]^{1/2}}. \quad (5)$$

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

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

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

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

For  $\text{Ga}_{0.8}\text{In}_{0.2}\text{As}$ , we find  $\tau_{alloy}^{-1}/\tau_{ac}^{-1} = 420/T$ , so that the rate of momentum relaxation for electron-alloy disorder scattering is higher than the rate of momentum relaxation for electron-acoustic phonon scattering.

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

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

From Equation (6), we show that, in the intrasubband scattering case, the scattering rate increases and the momentum relaxation time decreases as the transverse dimension of the wire decreases due to scattering from alloy-disorder. A formula similar to Eq. (6) has been obtained by Ando [20] and Bastard [21] for Q2D electron gas in this case.

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

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

where  $\langle \dots \rangle$  denotes the average, and is defined by the expression

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

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

$$f_0(E_{knl}) = \frac{(2\pi)^{1/2} \hbar m_e ab}{\gamma \delta (m^* K_B T)^{1/2}} \exp \left[ -\frac{n^2 E_n^0 + l^2 E_l^0}{k_B T} \right] \exp \left( -\frac{E_K}{k_B T} \right), \quad (9)$$

where

$$\gamma = \sum_n \exp \left( -\frac{n^2 E_n^0}{k_B T} \right), \delta = \sum_l \exp \left( -\frac{l^2 E_l^0}{k_B T} \right)$$

and  $n_e$  is the concentration of electrons. From this expression the Fermi energy can be identified as

$$\xi = K_B T \cdot \ln \left( \frac{\sqrt{2\pi} \hbar m_{1D}}{\gamma \delta (m^* k_B T)^{1/2}} \right). \quad (10)$$

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

$$\mu_{alloy}^{1D} = \frac{4eab\hbar^2}{\sqrt{2\pi} m^{*3/2} \Omega_0 (\delta V)^2 x (1-x) Z \gamma \delta (k_B T)^{1/2}} \sum_{nl} \exp \left( -\frac{E_{nl}}{k_B T} \right) \times \\ \times \left[ -B_{nn'l'l'}^2 \exp \left( \frac{B_{nn'l'l'}}{k_B T} \right) \text{Ei} \left( -\frac{B_{nn'l'l'}}{k_B T} \right) - B_{nn'l'l'} k_B T + (k_B T)^2 \right], \quad (11)$$

where

$$Z = 2(n'l') + n' + l' + 1/2,$$

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

Here,  $\text{Ei}(-x) = \int_{-\infty}^{-x} \frac{e^t}{t} dt$ .

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

$$\mu_{alloy}^{1D} = \frac{2eab\hbar^2}{\pi n_{1D} m^* \Omega_0 (\delta V)^2 x (1-x) Z} \sum_{nl} \frac{[\xi - (E_n + E_l)]^2}{[\xi - (E_n + E_l) + B_{nn'l'l'}]}. \quad (13)$$

Here, the Fermi energy  $\xi$  in this degenerate limit can be shown to be given by

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

where  $F(\eta)$  is the well-known Fermi integral [29].

In general, in the size quantum limit, where there is no approximation for  $f_0(E_{knl})$ , from Eqs. (6)–(8), the mobility can be written as

$$\mu_{alloy}^{1D} = \frac{4eab\hbar k_B T F_1 \left( \frac{\xi - 2E_n^0}{k_B T} \right)}{9\Omega_0 \pi m^* n_{1D} (\delta V)^2 x (1-x)} \quad (15)$$

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

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

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

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

If  $\mu_2$  is the alloy-scattering mobility in the Q2D system [23], then for a nondegenerate electron distribution,

$$\frac{\mu_{alloy}^{1D}}{\mu_{alloy}^{2D}} = \frac{3\pi^{3/2}ab(k_b T m^*)^{1/2}}{16\sqrt{2}d\hbar}, \quad (17)$$

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

$$\frac{\mu_{alloy}^{1D}}{\mu_{alloy}^{2D}} = \frac{27\pi^2 ab m^{*1/2} (\xi - 2E_a^0)}{16d\hbar} \quad (18)$$

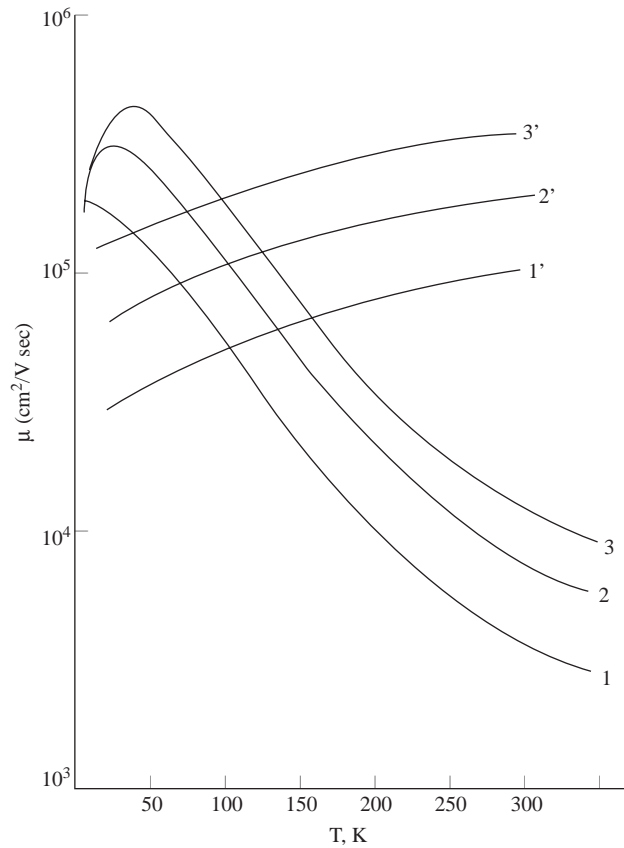
Equations (17), (18) show us that not only can a Q1D system exhibit greater mobility over a Q2D system, but that the enhancement depends on the temperature and on the cross-section of the quantum wire.

### 3. Numerical Analysis and Discussion

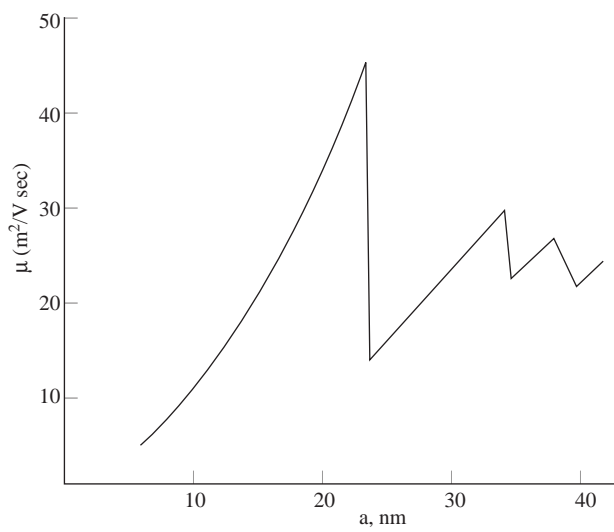
We have obtained general expressions for the momentum relaxation rate and electron mobility in a rectangular quantum wire for scattering due to alloy disorder. Electron mobility is expressed as a function of transverse dimensions of the wire and temperature. On the basis of these expressions, we have constructed Figures 1–3. For a numerical example, we consider the electron mobility in  $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$  quantum wire with alloy disorder scattering. The relevant values of physical parameters are taken to be  $\delta V = 0.6 \text{ eV}, \text{\AA}$

$$m^*(\text{Ga}_{0.47}\text{In}_{0.53}\text{As}) = 0.04m_0, \text{ and } \Omega_0 = \frac{5.87^3 \text{\AA}^3}{4}.$$

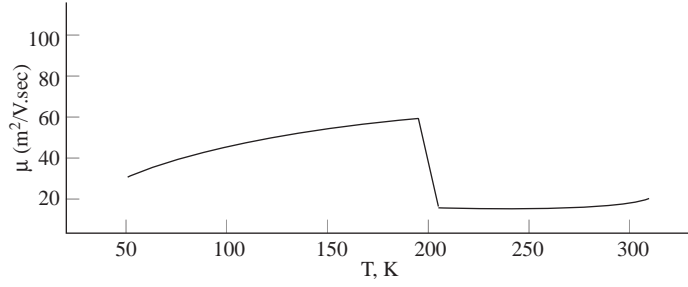
Figure 1 shows the mobility as a function of temperature due to alloy disorder scattering in the size quantum limit for various Q1D systems of selected transverse dimensions. For comparison, we also plot total mobility due to acoustic phonon, polar optic phonon and background impurity scattering for GaAs rectangular quantum wire found in the literature [2]. It is shown that the mobility becomes considerably enhanced as the cross-sectional area of the wire increases. It was predicted in [17] that the free-carrier absorption coefficient due to alloy-disorder scattering in Q1D structures decreases as transverse dimensions of the wire increases. This decrease in the free-carrier absorption coefficient explains the increase in the mobility predicted in our present results. As other scattering mechanisms (polar optical [2] and acoustic phonons [1, 2]), mobility-limited alloy disorder scattering also increases with increasing cross-sectional area of the wire.



**Figure 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 the wire ( $1'$ ,  $2'$ ,  $3'$ ). Curves 1, 2, 3, corresponds to the total electron mobility due to acoustic phonon, polar optic phonon and background impurity scattering in the Q1D systems [2]. We have chosen  $a= 10$  nm (1,  $1'$ ),  $a = 15$  nm (2,  $2'$ ),  $a = 20$  nm (3,  $3'$ ).



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



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

In Figure 2, we show the electron mobility as a function transverse dimension of the wire at 300 K. It is shown that the alternate increases/decreases of the mobility depending on the transverse dimensions of the quantum wire. It is also shown that because, no new intersubband scattering contributes, the mobility increases with increasing transverse dimension of the wire. At 300 K the electron distribution is classical and electrons are thermally distributed in energy roughly up to about  $k_B T$ . Consequently, the appearance of intersubband scattering due to alloy-disorder into the subband  $n$  is roughly determined by the condition

$$k_B T \geq E_{l1} \equiv E_l - E_1 \quad (19)$$

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

In Figure 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.

## Acknowledgements

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

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