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TEMPERATURE DEPENDENCE OF ELECTRON MOBILITY IN A FREE - STANDING QUANTUM WELL

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We have studied theoretically the low-field electron transport in a free-standing quantum well where the deformation potential scattering of electrons by acoustic phonons is the major mechanism of the electron relaxation. The quantization of acoustic phonons, their multisubband spectrum, and the exact form of the dilatational acoustic modes are taken into account. We have numerically solved the kinetic equation for electrons in the low electric field limit. At low lattice temperature the obtained electron distribution function has several peaks associated with scattering by different dilatational phonons. The electron mobility has temperature dependence similar to that described by the Bloch-Grüneisen formula, however we have obtained T^{-3} dependence of mobility in the low temperature region.

Key words: A. quantum well, thin films, D. electron-phonon interactions, phonons

The effect of acoustic phonon confinement on electron properties of free-standing structures, heterostructures and thin films is intensively studied both theoretically [1-5] and experimentally [6, 7]. There are several physical effects which are attributed to the quantization of the acoustic phonon spectrum. The peaks associated with confined acoustic phonons have been observed in the conductance of the quantum wires [6], luminescence spectra of $GaAs/AlGaAs$ quantum wells [7], and the Brillouin spectra of unsupported films [8].

In this paper we will consider the electron transport properties of a free-standing quantum well (FSQW) where the acoustic phonons are quantized in the normal to the surfaces of the quantum well direction. Such structures may be fabricated by various etching and lithographic techniques or by metal-organic epitaxy [8, 9] (see additional references in review [10]). We assume that the electron scatterings by acoustic phonons through the deformation potential is the major source of electron scatterings. The acoustic phonon modes in infinite solid slab are known from the field of acoustics [11]. There are shear waves, dilatational waves and flexural waves. We will specify the Cartesian coordinates such that axis z is perpendicular to the surfaces of the slab, axis x is in the direction of the phonon wave vector, axis y is perpendicular to x and z, and the origin is in the center of the slab. The vector of relative displacement for shear modes has only y component, thus, shear modes are similar to the transverse waves in bulk material and they do not interact with electrons through the deformation potential. The vectors of relative displacement for dilatational and flexural modes have both x anf z components and these types of modes differ by their symmetry. The Hamiltonians for electron interactions with dilatational and flexural phonons are given in Ref. [4]. We will use them to determine the transition probabilities for electron scatterings by confined phonons and to specify the collision integral of the kinetic equation for electron distribution function.

We have solved the kinetic equation numerically using the iterative technique in the low electric field limit where the electron distribution function may be represented as a sum of the equilibrium Fermi function and a small antisymmetric part. Though the kinetic equation is linear in respect to the applied electric field, it in nonlinear in respect to the scatterings by different acoustic modes and the Matthiessen's rule may not be used to determine the electron mobility. We have obtained the electron mobility by solving the kinetic equation and analyzed its temperature dependence.

We restrict our consideration by the case where only the first electron subband is occupied. Under these conditions only the dilatational phonons contribute to the electron-phonon scatterings through the deformation potential due to the symmetry selection rules [4] (if the potential energy for electrons is a symmetric function in respect to the mid-plane). The dilatational modes

are characterized by the mode number m and the in-plane wave vector $\mathbf{q}_{\|} = (q_x, 0)$; the corresponding frequency of the dilatational phonons are $\omega_m(\mathbf{q}_{\|})$. At $\mathbf{q}_{\|} = 0$ the function $\omega_m(\mathbf{q}_{\|})$ takes values from the following two sets

$$2n\pi\, s_t / a \quad \text{and} \quad (2n+1)\pi\, s_l / a\,,$$

where $n = 0, 1, 2, \ldots$, a is a width of the quantum well, and s_l and s_t are velocities of the longitudinal and transverse acoustic phonons in bulk material. We will nuber the dilatational modes in such a way that $\omega_m(\mathbf{q}_{\|}) < \omega_{m+1}(\mathbf{q}_{\|})$, and $m = 0, 1, 2, \ldots$. It follows from the above equations that only the zeroth mode has vanishing frequency at $\mathbf{q}_{\|} = 0$, all other modes have finite frequencies in the center of the Brillouin zone. The functions $\omega_m(\mathbf{q}_{\|})$ may have quite complex dependences on $q_{\|}$, particularly may have minima at $q_{\|} \neq 0$ [11]. Such minima result in formally infinite density of phonon states at appropriate energy and should have an effect on electron-phonon scatterings.

The electron probability density for the transition from initial state $\mathbf{k}_{\|}$ to the final state $\mathbf{k}'_{\|}$ due to an interaction with the dilatational phonon of mode m and in-plane wave vector $\mathbf{q}_{\|}$ may be determined from the Fermi golden rule. If we use the Hamiltonian for the electron scatterings given in [4] we obtain

$$W^{\left\{\substack{ab\\em}\right\}}_{\mathbf{k}_{\|}\to\mathbf{k}'_{\|}} = \frac{\pi E_a^2}{\mathcal{A}\rho}\, \mathcal{F}^{\left\{\substack{ab\\em}\right\}}(m,\, q_{\|})\times$$

$$\times\, \delta_{\mathbf{k}_{\|}\pm\mathbf{q}_{\|},\mathbf{k}'_{\|}}\, \delta(\varepsilon \pm \hbar\omega_m(\mathbf{q}_{\|}) - \varepsilon')\,, \qquad (1)$$

where

$$\mathcal{F}^{\left\{\substack{ab\\em}\right\}}(m,\, q_{\|}) = (n_{\mathbf{q}_{\|},m} + \frac{1}{2} \mp \frac{1}{2}) \mid F_{d,m} \mid^2 \omega_m^{-1}(\mathbf{q}_{\|})\times$$

$$\times \left(q_{t,m}^2 - {q_x}^2\right)^2 \left(q_{l,m}^2 + {q_x}^2\right)^2 \sin^2(\frac{a\, q_{t,m}}{2})\, \mathcal{G}(q_{l,m})\,, \quad (2)$$

$n_{\mathbf{q}_{\|},m}$ is the phonon occupation number, $q_{l,m}$ and $q_{t,m}$ are parameters determined from the solution of the dispersion equations for dilatational modes which denote the phonon wave vectors in z direction and take both real and pure imaginary values, $F_{d,m}$ is the dilatational phonon normalization constant [4]. Throught this paper the upper signs correspond to the phonon absorption, the lower signs correspond to the phonon emission. The overlap integral, $\mathcal{G}(q)$, is given by the formula

$$\mathcal{G}(q) = \left| \int_{-a/2}^{a/2} dz\; \psi^*(z)\, \psi(z)\, \cos(q\, z) \right|^2 ,$$

where $\psi(z)$ is the ground state for the one dimensional Schrödinger equation. If we use the electron wave functions for a rectangular infinitely deep quantum well, the overlap integral takes the form

$$\mathcal{G}(q) = \frac{32\,(1 - \cos\pi\tilde{q})}{\pi^2\,(\tilde{q}^2 - 4)}$$

where $\tilde{q} = a\, q/\pi$, and q is a real or a pure imaginary number.

To analyze the electron transport properties we will need scattering rates in the following form

$$\tau_G^{-1} = \sum_{\mathbf{k}'_{\|},m,\mathbf{q}_{\|},\beta} W^{\beta}_{\mathbf{k}_{\|}\to\mathbf{k}'_{\|}}\, G\,, \qquad (3)$$

where β is used to denote either *absorption* or *emission*, G is some given function which may depend on all variables over which we take the sum. We will also use $(\tau_G^{ab})^{-1}$ and $(\tau_G^{em})^{-1}$ which are defined in a similar way with the only distinction that we sum either only absorption terms or only emission terms. There is an obvious relation between them: $\tau_G^{-1} = (\tau_G^{ab})^{-1} + (\tau_G^{em})^{-1}$. If we employ the formulae for transition probabilities (1) we may obtain the following result for the scattering rates

$$\left(\tau_G^{\left\{\substack{ab\\em}\right\}}\right)^{-1} = \frac{E_a^2\, m}{2\pi\hbar^2\,\rho\, k_{\|}} \sum_m \int_0^{\infty} dq_{\|}\, \mathcal{F}^{\left\{\substack{ab\\em}\right\}}(m,\, q_{\|}) \frac{G}{\mid \sin\Psi \mid}\,, \qquad (4)$$

and the angle $\Psi \in [0, \pi]$ is a solutions of the equation

$$\cos\Psi = \frac{m\,\omega_m(q_{\|})}{\hbar\, k_{\|}\, q_{\|}} \mp \frac{q_{\|}}{2\, k_{\|}}\,.$$

Actually, the angle Ψ is the angle between $\mathbf{k}_{\|}$ and $\mathbf{q}_{\|}$. In the transition from Eq. (3) to Eq. (4) we have replaced the summation over a quasidiscrete variable by integration.

We have solved the electron transport problem for FSQW in the linear in respect to the drawing electric field approximation assuming that the electron scattering by confined acoustic phonons through the deformation potential is dominant. The electron distribution function (DF) $f = f(\mathbf{p})$ ($\mathbf{p}$ is the electron momentum) may be represented in the form

$$f = f_p^0 + \frac{\mathbf{f}_{1p}\,\mathbf{p}}{p}\,, \qquad (5)$$

where functions f_p^0 and $\mathbf{f}_{1p}$ depend on the absolute value of $\mathbf{p}$ and do not depend on its direction. The first term in the Eq. (5) is the symmetric part of DF and the second term is the antisymmetric part of DF. Because we are looking for the linear transport properties (formally the external force $F \to 0$) the symmetric part of DF is the equilibrium Fermi function. DF satisfies the kinetic equation with electron – confined acoustic phonon collision integral. We multiply the kinetic equation for DF defined by Eq. (5) by factor $\mathbf{p}/p$ and average it over the polar angle ϕ (vector $\mathbf{p}$ has components (p, ϕ) in the polar coordinate system an the polar axis is parallel to the applied field $\mathbf{F}$). In the end we get the following equation for the antisymmetric part of DF

$$\mathbf{F}\,\frac{\partial f_p^0}{\partial p} = \sum_{\mathbf{p}'} W_{\mathbf{p}\to\mathbf{p}'} \left[\frac{f_p^0}{f_{p'}^0}\,\mathbf{f}_{1p'}\,\cos\varphi - \frac{1 - f_{p'}^0}{1 - f_p^0}\,\mathbf{f}_{1p}\right], \qquad (6)$$

where $\mathbf{F}$ is the external force, $W_{\mathbf{p}\to\mathbf{p}'}$ is the electron

transition probability density defined by Eq. (1), φ is the angle between $\mathbf{p}$ and $\mathbf{p}'$. We are looking for the solution of Eq. (6) in the following form

$$\mathbf{f}_{1p} = -\tau_1(p)\,\mathbf{F}\,\frac{\partial f_p^0}{\partial p}. \tag{7}$$

Eq. (7) redefines the unknown function $\mathbf{f}_{1p}$ through the function $\tau_1(p)$. It will be shown below that $\tau_1(p)$ may be interpreted as the electron momentum relaxation time. From Eqs. (6), (7) we may obtain the following integral equation for the function $\tau_1(p)$

$$\tau_1(p)^{-1} = \sum_{\mathbf{p}'} W_{\mathbf{p}\to\mathbf{p}'} \left[1 - \frac{p'\cos\varphi}{p}\,\frac{\tau_1(p')}{\tau_1(p)}\right] \frac{1-f_{p'}^0}{1-f_p^0}. \tag{8}$$

To transform the sum in Eq. (8) to the integral and to include the explicit expression for the electron transition probability density due to scattering by confined acoustic phonons we use the result expressed by the formulae (3) and (4). We have solved Eq. (8) numerically using an iterative technique. The unknown function from the previous iteration has been used in the right hand side to obtain the updated function. The electron momentum relaxation time obtained in the test particle approximation has been used as an initial guess. The criteria for convergency was taken to be equal to 0.1% in the relative error. The iterative method converges fast in the case of a nondegenerate electron gas and in the case of a degenerate electron gas and high lattice temperatures ($T > 10\,K$, what corresponds to the energy of the acoustic phonon quantization). It took much more iterations (on the average, about 100) to obtain the convergence of the solution if the electron gas is degenerate and the lattice temperature is low ($T < 5\,K$). The numerical analysis was done for $GaAs$ FSQW of width $a = 100\text{Å}$ We took into account five of the lowest phonon modes; modes of the higher order make unnoticeable contribution to the scattering rate.

We will discuss here only the most interesting results of the numerical analysis related to the degenerate electron gas at low temperature. The Fermi energy is taken to be equal to $\varepsilon_F = 50\ meV$, what corresponds to the electron concentration $1.4 \times 10^{12}\ cm^{-2}$. The energy dependencies of f_1 for five lattice temperatures from $3\ K$ to $20\ K$ are displayed in Fig. 1.

The approximate symmetry of f_1 in respect to the Fermi energy $\varepsilon_F = 50\,meV$ follows from the principle of the detailed balance. The electron in a quantum state $\mathbf{k}'_{||}$ emits the phonon in a quantum state $\mathbf{q}_{||}$ and acquires a final state $\mathbf{k}_{||}$ with exactly the same probability as probability of the opposite process: electron in a quantum state $\mathbf{k}_{||}$ absorbs the phonon in a quantum state $\mathbf{q}_{||}$ and acquires a final state $\mathbf{k}'_{||}$. The local minima on the plots of Fig. 1 corresponding to the lattice temperatures $T = 3K$ and $T = 4.2K$ are related to the confined acoustic phonon scatterings. The minimum on the right of the Fermi energy is due to the phonon emission and on the left of the Fermi energy is due to the phonon absorption. The maximum wave vector of the acoustic phonons participating in the scatterings is approximately equal to doubled k_F and in our case constitutes $6 \times 10^6\,cm^{-1}$. If we restrict the length of the wave vector by this maximum value, the energies of the zeroth throgh the fourth mode acoustic phonons lies in the ranges $0 - 1.3meV$, $1.1 - 2.2meV$, $1.3 - 2.5meV$, $2.4 - 3.2meV$, $3.5 - 4.0meV$ [12]. These ranges overlap each other and minima of f_1 may not be associated with some particular mode; phonons of all five modes contribute to the electron scattering. The first mode make the main contribution, the scatterings by the zeroth and the second modes are also important, the influence of the third and higher modes is small [12]. The zeroth mode scatters electrons substantially weaker than the first mode because it has a surface bound character. It follows from the Eq. (8) that the electron scattering by different modes may not be calculated separately (as assumed by the Matthiessen's rule) and all the modes should be taken into account simultaneously.

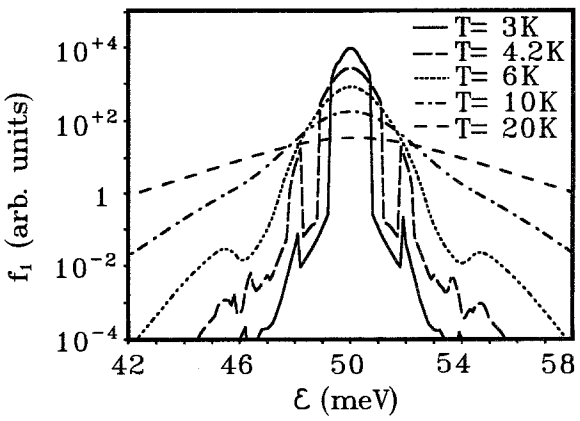

Figure 1: Function f_1 for five lattice temperatures displayed on the graph. $GaAs$ FSQW of width 100Å, $\varepsilon_F = 50meV$.

The electron mobility, μ, is expressed by the formula $\mu = e\tau_t/m$, where τ_t is the transport relaxation time obtained by averaging τ_1:

$$\tau_t = \frac{\int_0^\infty d\varepsilon\,(\varepsilon/T)\,\tau_1(\varepsilon)\,f_p^0(1-f_p^0)}{\int_0^\infty d\varepsilon\,f_p^0}. \tag{9}$$

We took integral (9) for series of temperatures and obtained temperature dependences of electron mobility. The temperature dependence of μ is shown in the Fig. 2. This result is very similar to the temperature dependence of μ of the 2DEG in $GaAs - Al_xGa_{1-x}As$ heterostructure observed in Ref. [13]. At high lattice temperatures the phonon population is much larger than unity and proportional to the lattice temperature. Therefore the rate of the electron scattering by phonons and the electrical resistivity are proportional to the lattice temperature. At low lattice temperatures the phonons

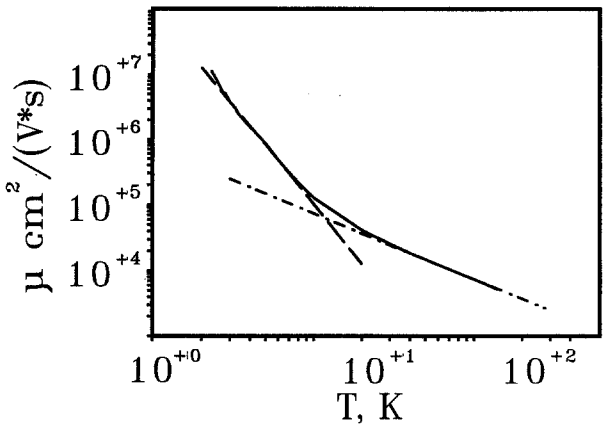

Figure 2: The electron low field mobility as a function of the lattice temperature.' The dashed line corresponds to T^{-3} dependence, the dash-dotted line corresponds to T^{-1} dependence; $GaAs$ FSQW of width $100\mathring{A}$, $\varepsilon_F = 50meV$.

with high energy will cease to be thermally exited, in our case the fourth mode will disappear at first, then the third mode and so on. The contribution of the frozen out phonons to the electron scattering is significantly reduced. In the case of metals this results in T^{-5} dependence of the electron mobility (Bloch-Grüneisen formula [14]). The same power dependence has been observed for 2DEG semiconductor quantum well [13]. We have obtained a smaller negative power (T^{-3}) for the temperature region ($3\ K < T < 8\ K$). For lattice temperatures $T < 3\ K$ the negative power becomes larger (see Fig. 2), however we did not proceed with our calculations below $T < 2K$ because the convergence of our computational algorithm deteriorates when temperature decreases and our model loose accuracy at very low temperatures since the piezoelectric potential scatterings become important.

It is interesting to note that though the momentum relaxation rate ${\tau_1}^{-1}$ has peaks near the Fermi energy, the transport relaxation time, τ_t, and the electron mobility, μ, do not have peaks associated with quantized acoustic phonons. Such peaks have been observed in the conduction variations of the electrically heated $AuPd$ FSQWs and FSQWIs [6]. However their origination lies in the nonlinear response of the electron – phonon system on the heating electric field.

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