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Emission and absorption of confined and interface optical phonons by electrons in the non-linear transport regime of a parabolic quantum wire

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Abstract. We present a detailed study of dissipation by electrons in the non-linear transport regime of harmonically confined quantum wires in GaAs/AlAs structures through emission and absorption of confined and interface optical phonons. An applied magnetic field perpendicular to the interfaces is used to modulate the natural harmonic frequencies in order to explore situations in and off resonance with the vibrational modes. Our results show that electrons absorb both confined phonons and interface phonons over wide angles and backwards, at low drift velocities. The emission occurs both forwards and backwards and dominates entirely for high drift velocities. The confined phonons play the dominant role in the dissipation, even for quantum wires inside thin quantum wells and with a magnetic field strength selected to make the harmonic levels in resonance with the AlAs-like interface mode.

1. Introduction

The process of emission and absorption of phonons by an electron gas driven by strong fields in low-dimensional semiconductor systems has been of considerable interest over the past few decades, due to their importance in semiconductor physics and electronics, and also in device applications [1]. The possibility of detecting the frequency and the angular dependence of phonon emission made necessary a theoretical analysis of the phonon spectrum emitted by electrons in semiconductors [2]. The generation of acoustic phonons from electrons in two- [3] and one-dimensional [4–7] semiconductor systems has been studied in detail. Recently, the emission and absorption of polar optical phonons by hot electrons was experimentally observed, and these processes are very sensitive to THz electromagnetic radiation [8–10]. Xu [2] has discussed the optical phonon emission spectrum obtained using hot electrons in a two-dimensional electron system under parallel magnetic fields. Currently, it is well known that, under high electric fields, electrons in a current are heated rapidly and dissipate energy mainly through the emission of phonons. In GaAs/Al$_x$Ga$_{1-x}$As microstructures, at low electron temperature (T_e below $\sim$40 K), the dominant process for cooling the electron system is the interaction with acoustic phonons. At higher temperature, this process is the Fröhlich interaction between electrons and longitudinal optical phonons, which exist as confined modes in GaAs, confined modes in Ga$_{1-x}$Al$_x$As, and interface modes.

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Here we treat the case of an electron gas in a quasi-one-dimensional channel which is created in a semiconductor heterostructure by holographic lithography [11]. The process starts with a laterally homogeneous modulation-doped $Ga_{1-x}Al_xAs$/GaAs heterojunction and confines the existing quasi-two-dimensional electron gas supplied by the shallow donor dopants in one additional direction by imposing a modulated voltage. The result is a collapse of the electron density in quasi-one-dimensional channels. The electron transport is diffusive but, due to the fact that the elastic scattering centres (impurities) are away from the electron gas, a very high mobility is obtained. For low electron densities the renormalized confining potential in the direction normal to the interfaces, originated by the modulated voltage, can be approximated by a harmonic potential [12–15]. In the present work we are interested in the non-linear transport of such a quantum wire under the action of an applied magnetic field perpendicular to the interfaces. The effect of the magnetic field, in this case, is to change the natural frequency of the harmonic confining potential, and renormalize the electron effective mass, as will be explained later. In general, the natural frequencies are of the order of a few meV. The application of a high magnetic field may change that frequency and cause it to approach the frequencies of the optical vibrational modes concerned, which are $\hbar\omega_{LO} = 36.2$ meV and $\hbar\omega_{TO} = 33.2$ meV for GaAs and $\hbar\omega_{LO} = 50.1$ meV and $\hbar\omega_{TO} = 44.9$ meV for AlAs. The averaged drift velocity of the centre of mass of the electron system, which is in the channel direction, depends on the applied voltage generating the current. The emission and absorption of phonons change with this drift velocity, but the system will respond differently for different values of the natural frequency (modified by the magnetic field) relative to the optical mode frequencies.

Beyond what has been done in previous work on phonon emission, we will: (i) consider the scattering by interface and confined optical phonon modes; (ii) consider the effect of electron drift, which should have a significant influence on the angular distribution of the emitted phonons; (iii) determine the transport properties, i.e. T_e, from transport equations rather than treating T_e as an input parameter. The model used here to represent a quantum wire (QW) is as follows: in the vertical (z-axis) direction an electron gas is structurally confined in a narrow quantum well of width L, which is a GaAs layer surrounded by thick AlAs layers; in the lateral y-direction, a modulated gate voltage creates a parabolic potential of natural frequency ω_0; the electron gas is free to move in the x-direction. This kind of structure is convenient to prepare and may be employed to investigate magneto-phonon resonances [7, 16] with a magnetic field $\boldsymbol{B}$ applied along the z-direction.

The process of dissipation through the scattering by optical modes in such QWs has to be treated taking into account the fact that, since the phonon frequencies of the two materials do not overlap, modes generated in one material cannot propagate into the other. Also, qualitatively different modes appear at the interfaces [17, 18]. Therefore, the dissipation by optical modes occurs due to the confined and interface modes instead of the usual Fröhlich scattering by bulk phonons. That feature is particularly important in harmonically confined QWs, due to the resonance that will necessarily occur. A magnetic field applied perpendicular to the interface modulates the natural harmonic frequency in a way that may bring the electron and the phonon systems into resonance. The consequences of the resonance for the non-linear resistivity of the QW were studied in a previous paper using the balance equation formalism [19]. On the basis of the transport properties, here we will further analyse the phonon emission and absorption spectra of these special vibrational modes, measured by the energy loss rate, i.e., the power transmitted to the lattice. The results are obtained for various magnetic field strengths, in order to cross regions in and off resonance with those modes. The electron density is assumed to be such that only the lowest subband of the confining potential in the z-direction is occupied (the first subband of the quantum well).

2. Non-linear transport in a harmonically confined quantum wire

In the past, the Lei and Ting balance equation (BE) formalism [20] has been applied successfully to describe the non-linear transport both in bulk materials and in semiconductor heterostructures. The steady state is determined, under the BE formalism, by two parameters, the steady-state average drift velocity, $\boldsymbol{v}_d$, and the effective electron temperature, T_e, satisfying the pair of coupled equations

$$-e\boldsymbol{E} + \boldsymbol{f}_{ph}(\boldsymbol{v}_d) = 0 \tag{1}$$

$$\boldsymbol{v}_d \cdot \boldsymbol{f}_{ph}(\boldsymbol{v}_d) + \omega(\boldsymbol{v}_d) = 0 \tag{2}$$

where $\boldsymbol{f}_{ph}(\boldsymbol{v}_d)$ and $\omega(\boldsymbol{v}_d)$ are the frictional force and the rate of energy loss per electron due to the inelastic interaction with phonons, respectively. In equation (1), for the sake of simplicity, we have neglected scattering by impurities and other defects. However, a complete treatment includes the residual resistivity, which is used as a given parameter identifying the sample and allowing one to obtain, as a function of the heat bath temperature, the pairs of v_d and T_e corresponding to the strength of the electric field applied, and, consequently, also the phonon resistivity:

$$\rho_{ph} = -\frac{\boldsymbol{v}_d \cdot \boldsymbol{f}_{ph}}{n^2 e^2 v_d^2}. \tag{3}$$

This formalism was applied recently in our QW model to obtain its non-linear resistivity. A resonance structure resulting from the calculation has been explained on the basis of inter-level scattering by GaAs and AlAs confined modes, and GaAs- and AlAs-like interface modes [19]. The energy of the electron state (m, k), reckoned from the first subbands, is given by

$$\epsilon_{m,k} = \epsilon_m + \frac{\hbar^2 k^2}{2m^*} \tag{4}$$

with

$$\epsilon_m = \epsilon_0 + \hbar\omega_0(m + 1/2) \tag{5}$$

where ϵ_0 is the first subband energy (in the z-direction), m^* is the effective mass, and ω_0 is the natural frequency of the harmonic potential.

The one-dimensional electron wave vector, $\boldsymbol{k}$, is assumed to be in the x-direction. In that case, the electron field operator is described as

$$\hat{\Psi}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{L}}} \sum_m \sum_{\boldsymbol{k}} \exp(\mathrm{i}kx)\phi_m(y)\zeta_0(z)c_{m,\boldsymbol{k}} \tag{6}$$

in which the wavefunction is normalized for electrons in a cube of length $\mathcal{L}$. $\zeta_0(z)$ is the ground-state eigenfunction for an electron in a well. $\phi_m(y)$ is the eigenfunction corresponding to level m of a harmonic oscillator:

$$\phi_m(y) = \left[\frac{1}{2^m m! \pi^{1/2} l_0}\right]^{1/2} H_m(y/l_0)\exp(-y^2/2l_0^2) \tag{7}$$

where $H_m(x)$ is the Hermite polynomial and $l_0^2 = \hbar/m^*\omega_0$. The operator $c_{m,\boldsymbol{k}}$ is the electron operator in the state corresponding to the harmonic level m and wavevector $\boldsymbol{k}$.

In the Landau gauge, a magnetic field applied in the z-direction modifies the one-electron eigenstates according to

$$\varepsilon_{m,k} = \left(m + \frac{1}{2}\right)\hbar\tilde{\omega} + \frac{\hbar^2 k^2}{2\tilde{m}} + \varepsilon_0 \tag{8}$$

$$\hat{\Psi}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{L}}} \sum_m \sum_{\boldsymbol{k}} \exp(\mathrm{i}kx)\phi_m(y - \tilde{y}_0)\zeta_0(z)c_{m,k}. \tag{9}$$

The natural frequency, the effective mass, and the Larmor radius are renormalized with respect to the magnetic field [21]:

$$\tilde{\omega} = \sqrt{\omega_c^2 + \omega_0^2} \qquad \tilde{m} = m^*\tilde{\omega}^2/\omega_0^2$$

$$\tilde{y}_0 = \tilde{b}\tilde{l}^2 k \qquad \tilde{l} = (m^*\tilde{\omega})^{-1/2}$$

respectively, with $\omega_c = eB/m^*$, $\tilde{b} = \omega_c/\tilde{\omega}$.

The optical phonon modes and Fröhlich interaction in this structure have been given by Mori and Ando [18]. Since only the first subband of the quantum well is considered, the half-space modes, which are confined to the thick AlAs layers, give a scattering potential which is odd in the z-coordinate, and, consequently, do not contribute to electron–phonon interaction.

There are four interface modes. They correspond to atoms vibrating in phase and in anti-phase at the two interfaces (symmetric modes (s) and anti-symmetric modes (a)) and modes associated either with the optical modes of GaAs (denoted by $-$) or with the optical modes of AlAs (denoted by $+$). The dispersion relations for these modes are obtained from the solutions of the relations connecting the real and imaginary parts of the dielectric function, for each wavevector in the (x, y) plane, $\boldsymbol{Q}_\parallel \equiv (q, Q_y)$:

$$\epsilon_1(\omega_{s\pm})\tanh(Q_\parallel L/2) + \epsilon_2(\omega_{s\pm}) = 0 \tag{10}$$

$$\epsilon_1(\omega_{a\pm})\coth(Q_\parallel L/2) + \epsilon_2(\omega_{a\pm}) = 0. \tag{11}$$

Only the symmetric modes contribute to the scattering in the first subband.

The rate of energy loss per electron in equation (2), due to confined and interface phonons, can be expressed as

$$\omega(v_d) = \sum_{m,m'} \sum_\lambda \int_0^{2\pi} \mathrm{d}\phi\ \mathcal{E}(m, m', \lambda, \phi) \tag{12}$$

and

$$\mathcal{E}(m, m', \lambda, \phi) = \int_0^\infty \mathrm{d}Q_\parallel\ Q_\parallel \Omega_{\boldsymbol{Q}_\parallel,\lambda} N(m, m', Q_\parallel, \lambda, \phi) \tag{13}$$

where $\mathcal{E}(m, m', \lambda, \phi)$ is the energy emitted due to the electron transition from harmonic state m to m', at azimuth angle ϕ, and for the phonon mode λ. Here λ stands for the vibrational mode. In the case of the confined modes, it is represented by an integer l, such that the wavevector in the z-direction is $Q_z = l\pi/L$. For the interface modes, λ is either $+$ or $-$. $N(m, m', Q_\parallel, \lambda, \phi)$ is the number of phonons generated for mode λ and wavevector $\boldsymbol{Q}_\parallel$. ϕ is the angle between the phonon wavevector $\boldsymbol{Q}_\parallel$ and the electron drift direction $\boldsymbol{v}_d$. $\Omega_{\boldsymbol{Q}_\parallel,\lambda}$ is the phonon energy of mode λ and wavevector $\boldsymbol{Q}_\parallel$. Using the BE formalism, it is straightforward to show that [19]

$$N(m, m', Q_\parallel, \phi, \lambda) = \frac{\mathcal{L}^2}{2\pi^2 n_e \hbar} \left| M^{0,0}_{m,m',\lambda}(\boldsymbol{Q}_\parallel) \right|^2 \Pi_2(m, m'; |q|, \Omega_{\boldsymbol{Q}_\parallel,\lambda} + \boldsymbol{q}\cdot\boldsymbol{v}_d)$$
$$\times \left[n\left(\frac{\Omega_{\boldsymbol{Q}_\parallel,\lambda}}{T}\right) - n\left(\frac{\Omega_{\boldsymbol{Q}_\parallel,\lambda} + \boldsymbol{q}\cdot\boldsymbol{v}_d}{T_e}\right) \right]. \tag{14}$$

In the above equation, $\Pi_2(m, m'; |q|, \Omega_{Q_\parallel,\lambda} + \boldsymbol{q} \cdot \boldsymbol{v}_d)$ is the imaginary part of the polarization function [22], and $n(\epsilon)$ is the Bose distribution function. $M^{0,0}_{m,m',\lambda}(\boldsymbol{Q}_\parallel)$ is the matrix element of the electron–phonon interaction, i.e., the $\boldsymbol{Q}$-component of the scattering potential $M_\lambda(\boldsymbol{Q})$ [23]:

$$\left|\mathbf{M}^{0,0}_{m,m',\lambda}(\boldsymbol{Q}_\parallel)\right|^2 = \left|J_{m',m}(u)\right|^2 \left|I_{0,0}(Q_z)\right|^2 |M_\lambda(\boldsymbol{Q})|^2 \tag{15}$$

$$I_{0,0}(Q_z) = \int_{-\infty}^{\infty} \mathrm{d}y \;\; \exp(\mathrm{i}Q_z z)\zeta_0^*(z)\zeta_0(z) \tag{16}$$

and

$$\left|J_{m,m'}(u)\right|^2 = \left|\int_{-\infty}^{\infty} \mathrm{d}y \;\; \exp(\mathrm{i}Q_y y)\phi^*_{m'}(y)\phi_m(y)\right|^2 \tag{17}$$

that is

$$\left|J_{m,m'}(u)\right|^2 = \frac{m!}{m'!}\mathrm{e}^{-u}u^{m'-m}\left[L_m^{m'-m}(u)\right]^2 \qquad \text{for } m \leqslant m'. \tag{18}$$

where $u = \tilde{l}^2(Q_y^2 + \tilde{b}^2 q^2)/2$ and $L_m^{m'}(u)$ is a Laguerre polynomial.

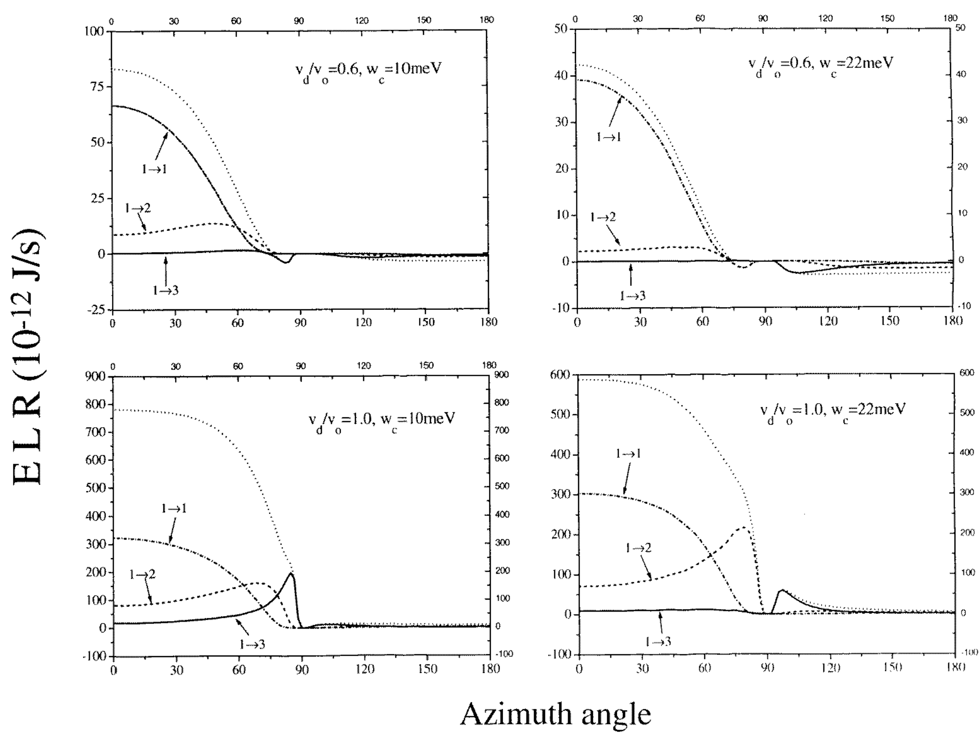

Figure 1. Rates of energy loss due to the scattering by GaAs confined modes, in watts/electron, as a function of the azimuth angle, for a quantum wire in a GaAs layer of width 100 Å and with 10^5 electrons cm^{-1}. The dotted lines give the total energy loss rate, and the other lines give the partial contributions due to the transitions indicated.

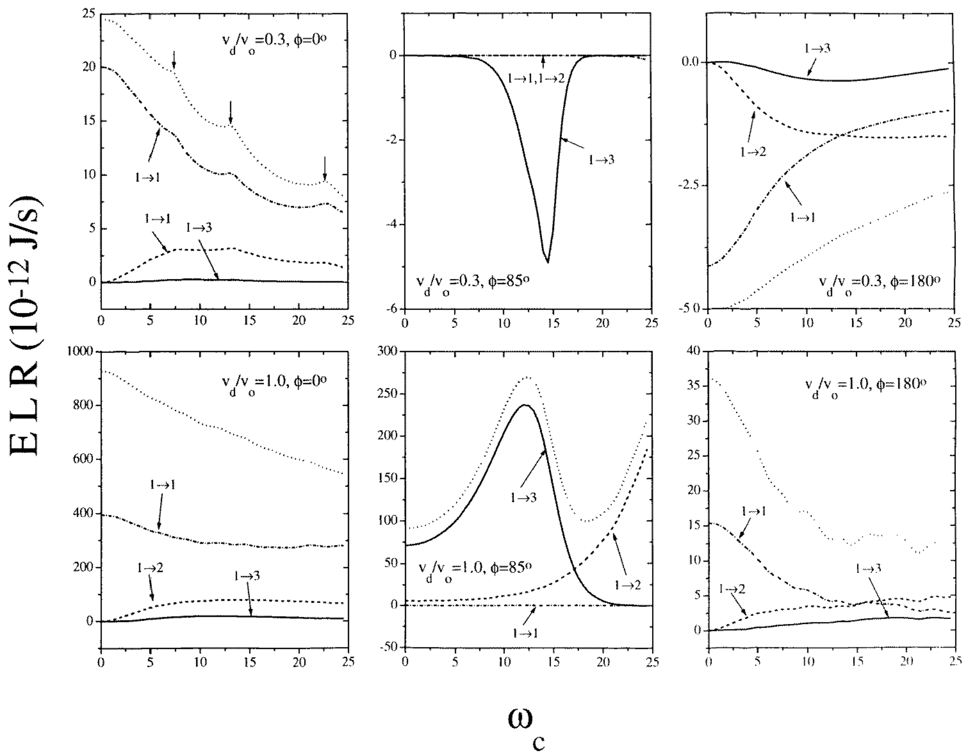

Figure 2. Rates of energy loss due to confined GaAs modes, for the same quantum wire, calculated for different azimuth angles (0°, 85°, and 180°) and in the low- ($v_d/v_0 = 0.3$) and high- ($v_d/v_0 = 1.0$) drift-velocity regimes, as functions of the magnetic field strength, given by the cyclotron frequency ω_c.

3. Results and comments

We have performed our calculation for a QW with $\omega_0 = 10$ meV, $n_e = 10^5$ electrons cm^{-1}, and a heat bath temperature of 77 K. (For the sake of simplicity, $\hbar = 1$ will be used in the following discussion.) Electron temperatures T_e corresponding to the results are determined from the balance equations (equation (1) and (2)) as in reference [19]. We have obtained good convergence in all cases by including the first six harmonic levels. In figure 1 we show the energy loss rate (ELR) for energy loss due to the scattering by GaAs confined phonons for a GaAs width of 100 Å. The total ELR (dotted curve) and a few intra- and inter-level transitions are shown as functions of the azimuth angle ϕ. In the plots on the left, we made $\omega_c = 10$ meV. Since we have chosen $\omega_0 = 10$ meV, that choice of the magnetic field strength makes the transition involving the first and the third levels very close in energy to the GaAs confined mode. We have calculated the ELR for $v_d = 0.6v_0$ and $v_d = 1.0v_0$, where v_0 is the GaAs optical velocity scale, i.e., $\Omega_{\mathrm{GaAs}LO} = mv_0^2$. Notice that the emission of phonons corresponds to positive ELR, and the absorption to negative values. The most important contribution to the forward emission (small values of ϕ) comes from the $1 \to 1$ transition. As v_d/v_0 approaches 1.0, several other transitions become important (that is why we have to include six harmonic levels to obtain a good convergence). For that velocity (deep into the non-linear regime) the emission is very strong, dominating completely over

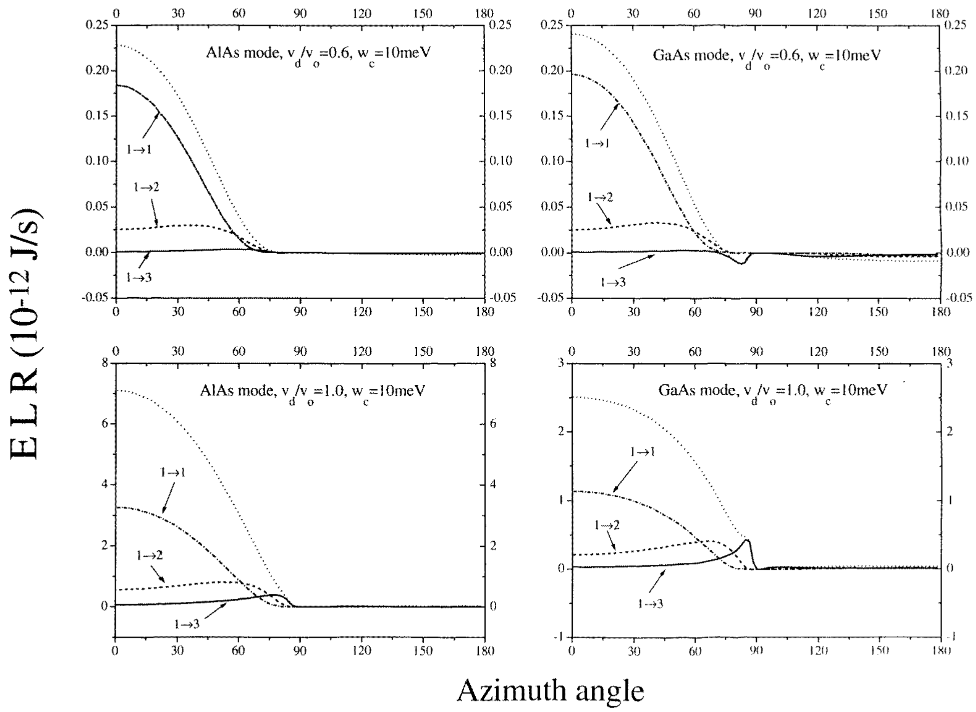

Figure 3. Rates of energy loss due to the interfaces modes, for the same quantum wire, as functions of the azimuth angle, with the magnetic field strength of $\omega_c = 10$ meV, in resonance with the GaAs-like interface modes.

the absorption. When the electron drift energy is much lower than the optical phonon energy (e.g., $v_d = 0.6v_0$), the electron emits phonons forward only, with angles less than 75°, while it absorbs phonons over wide angles forward and backward, near 90°, involving only small q-wavevectors over a large range of $Q_\parallel$. The absorption is determined by the $1 \to 3$ transition, most of all. This characteristic of absorbing phonons forward over a wide angle (near 90°) stems from the cooling effect predicted by the Lei–Ting balance equation [19, 24]. Once the electron drift velocity approaches the optical phonon velocity, the electron will emit phonons both forward and backward. In the case of resonance, in particular, the electron will strongly emit phonons in wide-angle forward directions. Since wide-angle phonon emissions and absorptions are strongly determined by the harmonic resonance status, we believe that measurements of this wide-angle phonon emission and absorption can provide more information about the phonon resonances. The other two plots on the right show the case where $\omega_c = 22$ meV, a situation that is off resonance, although the difference in energy between the first and third levels, in that case, matches the energy of the AlAs confined modes.

In figure 2 the ELR for loss due to scattering by the same confined modes is calculated as a function of the magnetic field strength expressed in terms of the cyclotron resonance ω_c, for a structure with a GaAs layer width of 100 Å. The upper three plots, for $v_d/v_0 = 0.3$, are performed for the angles 0°, 85°, and 180°. The lower plots show, for the same angles, the ELR for $v_d/v_0 = 1.0$. We observe a complete change in the pattern. Here we show the results for $v_d/v_0 = 0.3$ instead of for $v_d/v_0 = 0.6$ to represent the case of low speed,

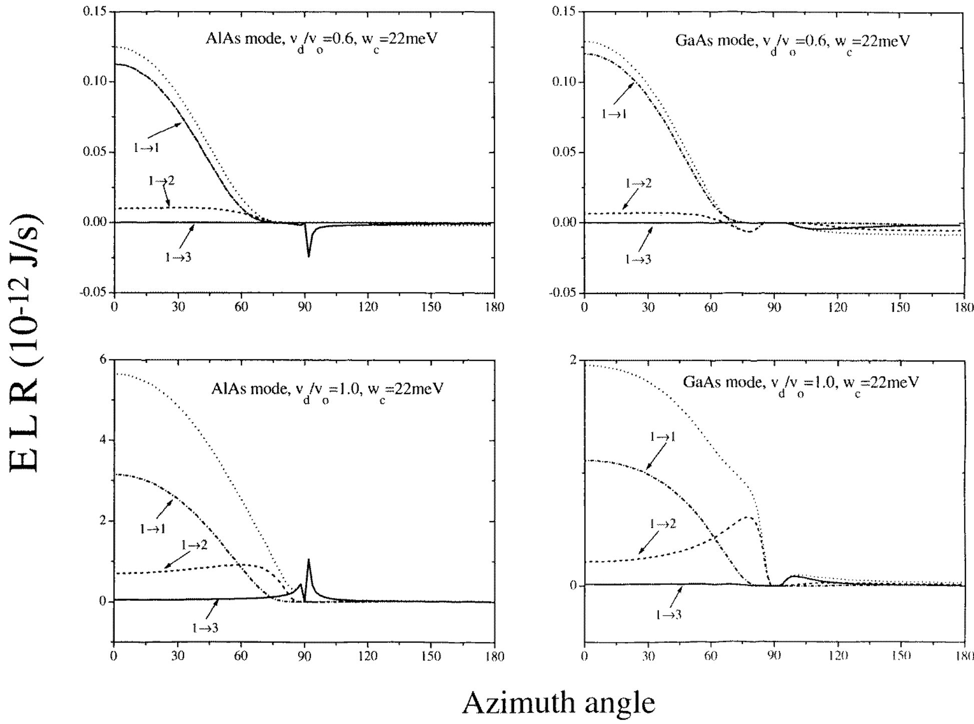

Figure 4. As before, but with $\omega_c = 22$ meV, in resonance with the AlAs-like interface modes.

because, although they have similar patterns, the former gives a sharper and more detailed structure. As discussed in reference [19], the cooling effect appears when $v_d/v_0 < 0.6$ in the case in which the Fröhlich interaction dominates the electron relaxation mechanism, and the phonon emission and absorption by the electron gas show the low-speed pattern over this range of drift velocity. The low-speed forward ($\phi = 0°$) ELR is dominated by emission, mainly the $1 \to 1$ transition, and shows a structure like that observed in the low-speed resistivity [19]. The emission peaks, denoted by arrows to the total curve, come from the increase of the electron temperature when magneto-phonon resonance occurs, corresponding to peaks of resistivity. These three peaks correspond to the $1 \to 4$ confined mode transition ($\omega_c = 6.7$ meV), the $1 \to 3$ confined mode transition ($\omega_c = 14$ meV), and the $1 \to 3$ AlAs interface mode transition ($\omega_c = 23$ meV), respectively. At wide angles (near 85°) a strong absorption peak appears, determined by the resonance with the $1 \to 3$ transition. The backward ($\phi = 180°$) ELR—the third plot in the upper section—is dominated entirely by absorption, showing an important contribution of the $1 \to 1$ transition. At high speeds, as shown in the lower plots, the emission dominates, and even the absorption peak for wide angles changes into an emission peak.

In figure 2, we notice that both the emission forwards and the absorption backwards due to the intrasubband $1 \to 1$ transition decrease with the magnetic field, because electrons concentrate into the first subband and the electron gas. Phonon emission or absorption due to the intersubband $1 \to 2$ transition, on the other hand, increases with the increase of the magnetic field before the first resonance $\omega_c = 6.7$ meV, because of the increase of the electron temperature. It is also important to notice that the resonance position changes with

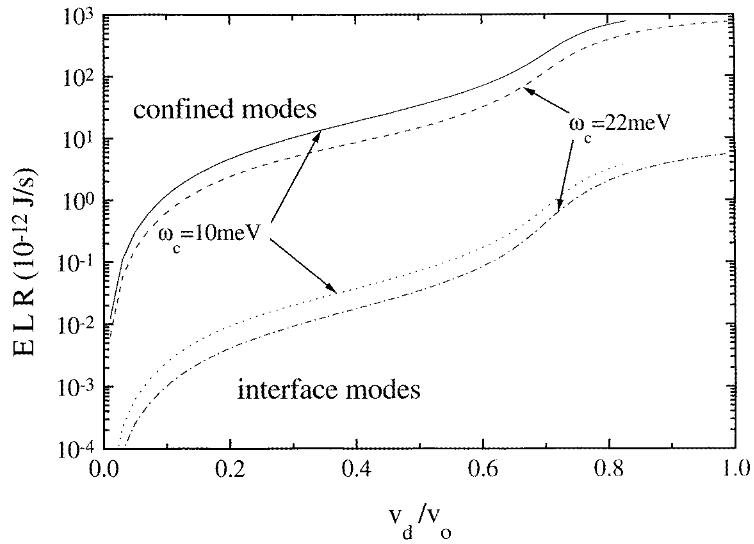

Figure 5. The ELR for the confined and interface modes calculated for $\omega_c = 10$ meV and $\omega_c = 22$ meV.

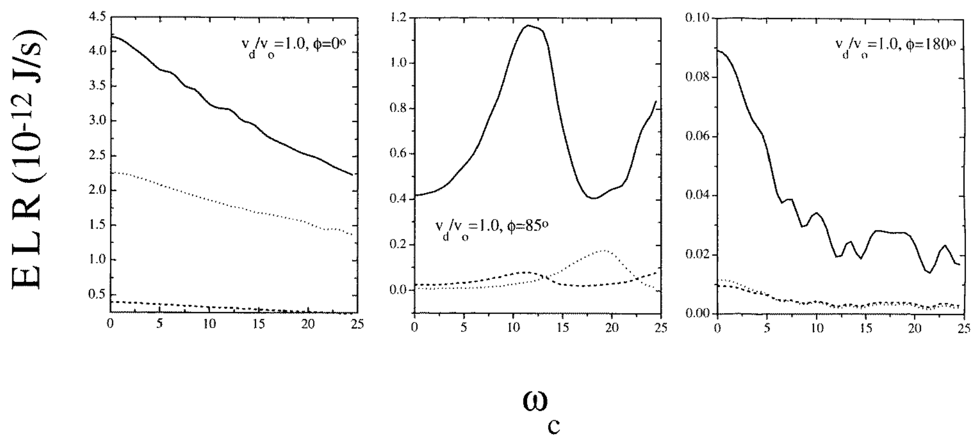

Figure 6. The ELR for a QW with a GaAs layer width of 40 Å as a function of the magnetic field, $v_d/v_0 = 1.0$, and for the azimuth angles 0°, 85°, and 180°.

different electric fields and angles of phonon detection.

The same calculations have been performed for the interface modes. Figure 3 shows the ELR for both the GaAs- and AlAs-like interface modes in a GaAs layer of 100 Å, and for $\omega_c = 10$ meV. It is worthwhile to call attention to the fact that, even at $v_d = 0.6v_0$, a small absorption peak appears near $\phi \simeq 90°$ for the GaAs-like mode, as a signature of the resonance with that mode. In figure 4, for $\omega_c = 22$ meV, the equivalent peak appears in the AlAs-like mode. As before, for both frequencies, the emission dominates over the absorption at high speeds.

Figure 5 shows the total ELR for confined and interface modes as functions of the electron drift velocity v_d. The calculation has been performed with a GaAs width of 100 Å and a natural frequency $\omega_0 = 10$ meV, and for $\omega_c = 10$ meV and $\omega_c = 22$ meV. Here we can see that the ELR increases rapidly with v_d. We can see, however, that the total rate of energy loss due to the interface modes is small as compared with the contribution due to the confined modes. In order to see whether this behaviour is restricted to wide quantum wells, we have also performed a complementary calculation for a QW with the same natural frequency and with electron density as before, for $v_d/v_0 = 1.0$, but with a GaAs layer width of 40 Å. As is well known, interface modes play a more important role in narrow wells. However, a GaAs/AlAs quantum well undergoes a type-I–type-II transition for a width near 37 Å. Just before this width is reached, Γ–X hybridization becomes relevant [25]. For this reason, we wanted to see whether, in narrow wells, such as one with $L = 40$ Å, the ELR behaviour was different from that of our calculations for $L = 100$ Å shown in the previous figures. These results for the ELR, as a function of the magnetic field strength, are shown in figure 6. The solid lines are the ELRs for loss due to the confined modes; the dotted and dashed lines are due to interface modes, for AlAs and GaAs, respectively. Again, emission dominates over the absorption, and the contributions due to the confined modes are more important than those of the interface modes. Among these, the AlAs-like mode dominates the forward emission. Different positions of the emission peak at wide angles correspond to the resonance with the GaAs-like mode (around 10 meV), and with the AlAs-like mode (around 22 meV). Therefore, no remarkable difference in the ELR pattern occurs for so thin a quantum well.

In conclusion, we have studied the angle and magnetic field dependences of the phonon emission and absorption by electrons in a harmonically confined GaAs/AlAs quantum wire. Our calculation indicates that the rate of electron energy loss due to scattering with optical modes increases with the drift velocity, as it should, as it is the most important mechanism for transferring energy to the lattice. The transfer through confined GaAs modes is much more significant than that through interface modes. At low drift velocities (the linear regime), electrons emit phonons forwards and absorb phonons backwards and forwards over wide angles. At high drift velocities (the non-linear regime), especially when they are travelling at approaching or more than the optical velocity, electrons only emit phonons both forward and backward. At intermediate velocities a small absorption peak, due to the confined GaAs mode (at $\omega_c = 15$ meV, for a QW with the parameters used), and two others that are much smaller, due to the interface modes (at $\omega_c = 10$ and 22 meV), could be detected if a sensitive directional measurement could be performed, corresponding to scatterings over wide angles.

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