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Asymmetric inter-subband phonon scattering associated with the intra-collisional field effect in one-dimensional quantum wires

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Abstract. The rates of scattering by confined longitudinal optical phonons in one-dimensional quantum wires are calculated by taking into account the intra-collisional field effect (ICFE) associated with high electric fields. It is shown that the scattering rate becomes asymmetric with respect to the direction of the electron propagation due to the ICFE. In particular, the energy dependence and strength of the backward scattering are greatly modified by the ICFE. Asymmetry in the scattering rates is noticeable even when multi-subband scatterings are significant in thick quantum wires.

1. Introduction

Intense research activities have been devoted to high-temperature carrier transport in low-dimensional structures because of their potential for device applications. In particular, quasi-one-dimensional structures, owing to the dramatic change of the phonon scattering rates associated with the one-dimensional (1-D) density of states, are expected to show mobility much higher than that in bulk [1]. Since the electron-transport properties in 1-D quantum wires are dominantly controlled by low-energy electrons (up to a few hundreds of meV), the details of the scattering rates employed in the electron-transport analyses are rather sensitive to the results [2, 3].

In the present paper, the rates of electron scattering via confined longitudinal optical (LO) phonons in GaAs 1-D quantum wires are investigated under high electric fields. Unlike previous investigators [1–3], we have taken into account the intra-collisional field effect (ICFE), which is associated with the electron acceleration or deceleration due to the external electric field during the duration of the collision with phonons [4, 5]. The ICFE has been extensively studied for 3-D bulk structures by several groups [6–11]. The predicted electric field strengths under which the ICFE is supposed to be significant are extremely strong and vary from several tens of kV cm^{-1} to MV cm^{-1}. As we have pointed out, on the other hand, inclusion of the ICFE could be essential in low-dimensional structures even under *moderately strong* electric fields [12]; since the ICFE is most significant when the phonon's momentum is parallel or anti-parallel to the electric field, the ICFE in 1-D structures where the electron motion is restricted to being along the electric field direction could be *always* effective in each scattering event with phonons.

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2. The scattering rate and spectral density

We consider ideal rectangular 1-D quantum wires with an infinitely deep potential well in the transverse (y- and z-) directions. The electron wavefunction in a 1-D quantum wire is then expressed by

$$\langle \boldsymbol{r}|\boldsymbol{k}, l, m\rangle = \frac{1}{\sqrt{L_x}} \mathrm{e}^{\mathrm{i}kx} \sqrt{\frac{2}{L_y}} \sin\left(\frac{l\pi y}{L_y}\right) \sqrt{\frac{2}{L_z}} \sin\left(\frac{m\pi z}{L_z}\right) \tag{1}$$

with $l = 1, 2, \ldots$ and $m = 1, 2, \ldots$. Here, $\boldsymbol{k}$ is the electron wave-vector, and L_x, L_y, L_z are the lengths of the rectangular quantum wire along the x-, y-, z-directions, respectively. In the present study, we have employed the Fröhlich polar scattering with the confined LO phonons, which is the dominant scattering channel in GaAs 1-D quantum wires [2, 3]. The confined electron–LO-phonon scattering rate for the electron with $\boldsymbol{k}$ in the subband (l, m) is evaluated from the Fröhlich Hamiltonian along with Fermi's golden rule [13, 14]:

$$\begin{aligned} w_{\mathrm{LO}}^{e/a}(\boldsymbol{k}, l, m) = {} & \frac{e^2}{8\pi\varepsilon_0}\left(\frac{1}{\kappa_\infty} - \frac{1}{\kappa_0}\right) \sum_{l', m'} \int_{-\infty}^{\infty} \mathrm{d}q_x\ \omega_q I_{1\mathrm{D}}(q_x, L_y, L_z) \\ & \times \left(N_{\boldsymbol{q}} + \frac{1}{2} \pm \frac{1}{2}\right) \delta[E(k \mp q_x, l', m') - E(k, l, m) \pm \omega_q] \end{aligned} \tag{2}$$

where the upper (lower) sign corresponds to the emission (absorption) process, $\boldsymbol{q}$ is the phonon wave-vector, e is the magnitude of the electron charge, ε_0 is the permittivity of vacuum, κ_0 (κ_∞) is the dielectric constant at low (high) frequency, $N_{\boldsymbol{q}}$ is the phonon occupation number, $\omega_{\boldsymbol{q}}$ is the LO-phonon energy (=36 meV for GaAs), and $E(k, l, m)$ is the electron energy. Notice that we use the units of $\hbar = 1$ throughout the paper. The structure factor $I_{1\mathrm{D}}(q_x, L_y, L_z)$ is given by

$$I_{1\mathrm{D}}(q_x, L_y, L_z) = \frac{(2\pi)^2}{L_y L_z} \left\{ \sum_{p,\, q\, =\, 1,\, 2,\, \ldots} \frac{4F_p(l, l')F_q(m, m')}{q_x^2 + (p\pi/L_y)^2 + (q\pi/L_z)^2} \right\}^2 \tag{3}$$

with

$$F_p(l, l') = \frac{1}{2\pi} \left\{ \frac{1 - (-1)^{l+l'-p}}{l + l' - p} + \frac{1 - (-1)^{l-l'+p}}{l - l' + p} - \frac{1 - (-1)^{l+l'+p}}{l + l' + p} - \frac{1 - (-1)^{l-l'-p}}{l - l' - p} \right\}. \tag{4}$$

The central quantity which allows us to incorporate the ICFE is the spectral density in the transition probability; the conventional spectral density given by the energy-conserving delta function in equation (2) is replaced by that obtained from the quantum kinetic equation [7]. The spectral density $S(k_F, \boldsymbol{q})$ under the constant electric field F is given by

$$S(k_F, \boldsymbol{q}) = \frac{1}{\pi} \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{-\Gamma_k \tau} \cos[(E(k_F - \eta q_x, l', m') - E(k_F, l, m) + \eta\omega_{\boldsymbol{q}})\tau] \tag{5}$$

with $k_F = k + eF\tau$. Here, it is assumed that the electric field is directed to the negative x-direction. $\eta = 1$ (-1) corresponds to phonon emission (absorption). $\Gamma_{\boldsymbol{k}}$ is the total LO-phonon scattering rate and we have assumed that the time correlation between two successive scatterings is destroyed by a collision with phonons. Notice that when the electron lifetime is infinite ($\Gamma_{\boldsymbol{k}} = 0$) and the electric field is suppressed ($F = 0$), equation (5) correctly reduces to the usual energy-conserving delta function.

The spectral densities of phonon emission evaluated from equation (5) for the electron moving parallel ($\boldsymbol{k} < 0$) or anti-parallel ($\boldsymbol{k} > 0$) to the electric field of $F = 500$ V cm^{-1}

are shown in the insets to figure 1. As is already well known [4, 5], the ICFE essentially has two effects: it broadens the energy-conserving delta function and skews the energy detuning (zero point). More importantly, however, the direction to which the spectral density is skewed is dependent on the direction of the electron motion. When the electron propagates against the electric field ($\boldsymbol{k} > 0$), the spectral density shifts to the positive direction, and vice versa. Their physical origin will be discussed in the next section. Both the energy broadening and the skewness due to the ICFE are directly related to the strength and direction of the electric field, and their magnitude is given by

$$\Delta_F \approx \left[\frac{e|\boldsymbol{q}\cdot\boldsymbol{F}|}{2m^*}\right]^{1/2} \tag{6}$$

where m^* is the electron effective mass. Since the spectral densities shown in the insets to figure 1 are not positive definite, evaluation of the scattering rates in terms of the *oscillating* spectral density given by equation (5) requires enormous CPU time [12]. We have thus approximated the spectral density by the Gaussian form with the width and shift given by Δ_F in the present calculations. Similarly, the gaussian spectral density has been employed in the analyses of collisional broadening by Briggs *et al* [15]. The approximated spectral densities are also plotted as dotted lines in the insets to figure 1.

3. Results and discussion

The confined Fröhlich LO-phonon scattering rates under various electric fields at temperature $T = 300$ K are shown in figures 1 and 2 for thin ($L_y = 7$ nm and $L_z = 10$ nm) and thick ($L_y = 30$ nm and $L_z = 30$ nm) quantum wires, respectively. The LO-phonon scattering rates from the lowest subband to the first 20 subbands including the intra-subband scattering have been evaluated. Because of the energy broadening in the spectral density, the divergence of the scattering rate associated with the singularity in the 1-D density of states is removed. Notice that the scattering rates for $F = 0$ V cm^{-1} coincide with those obtained from Fermi's golden rule. It is thought that the error incurred by the infinite potential barrier employed in the quantum wires would not be crucial in the present results; the finite barrier height in a *real* quantum wire would lead to the leaking of the electrons confined in the wire and this is in some respects equivalent to the inclusion of the inter-subband scatterings in this study.

More importantly, the ICFE makes the scattering rates asymmetric with respect to the direction of the electron motion. That is, the first peak in the scattering rates for the thin quantum wire (see figure 1) splits into two peaks depending on the direction of the electron motion. Since this peak corresponds to phonon emission, asymmetry is ascribed to the shift of the energy detuning in the spectral density, as shown in the insets to figure 1, and can be explained as follows. When an electron moves against the electric field ($\boldsymbol{k} > 0$), it gains energy from the electric field during the duration of the collision with the phonons. Therefore, it can emit an LO phonon even if the electron energy just before the scattering is smaller than the threshold energy for phonon emission. In other words, the phonon energy is effectively reduced when the electron moves against the electric field and the peak of the scattering rate shifts to the lower-energy side. On the other hand, when it moves along the electric field ($\boldsymbol{k} < 0$), an electron loses its energy. Thus, the phonon energy is effectively increased and the peak of the scattering rate shifts to the higher-energy side.

For the thick quantum wire where multi-subband scatterings are significant (see figure 2), many peaks in the scattering rates from Fermi's golden rule are smeared out and disappear in high-energy regions due to the energy broadening associated with the ICFE. However, asymmetry in the low-energy regions is still noticeable. Since the electron-transport

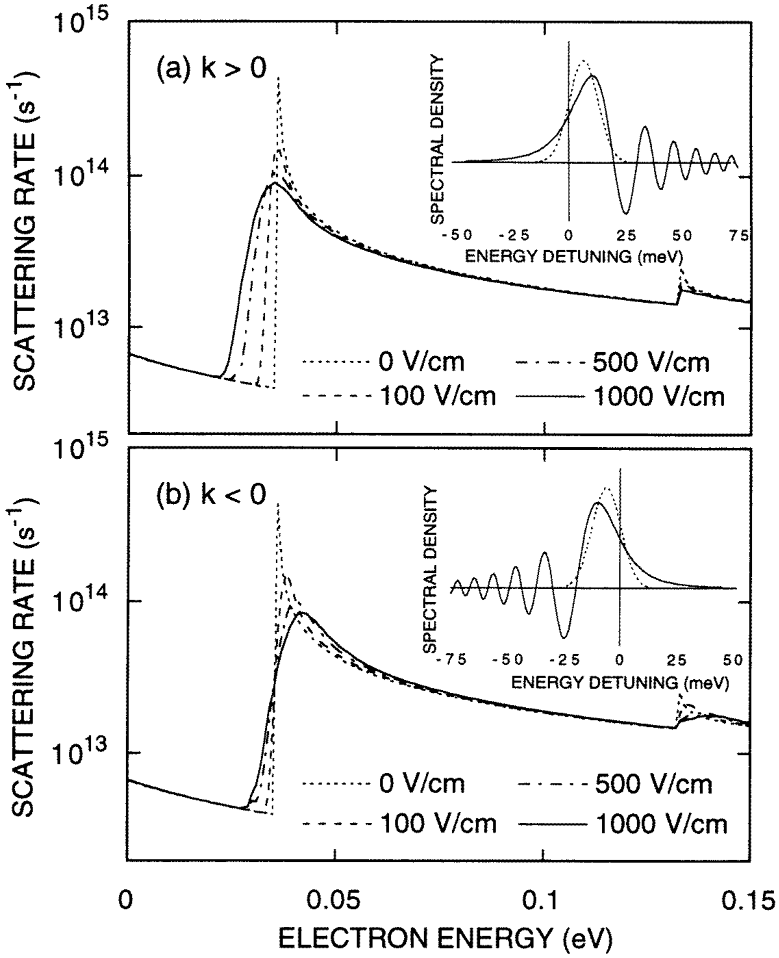

Figure 1. Electron–LO-phonon scattering rates for the electron propagating in the (a) positive ($\boldsymbol{k} > 0$) and (b) negative ($\boldsymbol{k} < 0$) directions in the thin quantum wire ($L_y = 7$ nm and $L_z = 10$ nm) under $F = 0$, 100, 500 1000 V cm^{-1} and for $T = 300$ K. The scatterings from the lowest subband to the first 20 subbands (including the lowest subband) are included. The electron energy is measured from the bottom of the lowest subband. Insets: electron spectral densities as a function of energy detuning for the electron with (a) $\boldsymbol{k} > 0$ and (b) $\boldsymbol{k} < 0$ under $F = 500$ V cm^{-1} (solid lines). The dotted lines represent the approximated spectral densities employed in this study.

properties in quantum wires are dominantly controlled by the electrons in such low-energy regions, the ICFE could be still effective on transport properties even if the sizes of the 1-D quantum wires are rather large.

In order to investigate the effects of asymmetric scattering rates on the transport properties, the forward- and backward-scattering rates under $F = 1000$ V cm^{-1} for the thick quantum wire are plotted in figure 3. Again, the forward and backward scatterings are modified by the ICFE and become dependent on the direction of the electron's motion. Since the magnitude of the phonon's wave-vector involved in the backward scattering is always greater than that in the forward scattering, the ICFE is most effective in the backward

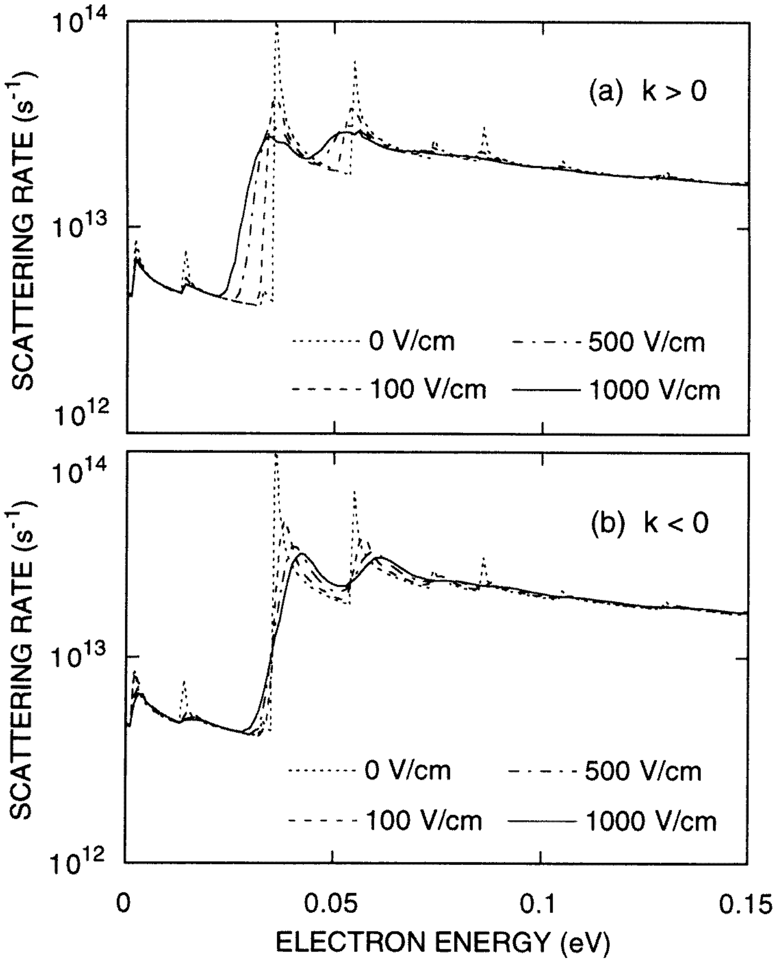

Figure 2. Electron–LO-phonon scattering rates for the electron propagating in the (a) positive ($\boldsymbol{k} > 0$) and (b) negative ($\boldsymbol{k} < 0$) directions in the thick quantum wire ($L_y = 30$ nm and $L_z = 30$ nm) under $F = 0$, 100, 500 1000 V cm^{-1} and for $T = 300$ K. The scatterings from the lowest subband to the first 20 subbands (including the lowest subband) are included. The electron energy is measured from the bottom of the lowest subband.

scattering. Indeed, the backward scattering greatly changes its energy dependence and strength, i.e., the backward scattering for the electron with $\boldsymbol{k} > 0$ becomes active with energy below the threshold energy of phonon emission (=36 meV). In addition, the strength of the backward scattering for the electron with $\boldsymbol{k} < 0$ is reduced compared with the semi-classical rate. As a result, it is thought that the electron velocity would be reduced when the ICFE was taken into account. We would like to stress that the drift-velocity reduction is expected even when the dimension of the quantum wires is rather large as in the present thick quantum wire, so multi-subband scatterings are significant. This is in marked contrast to the cases of *low-temperature* transport, in which the phase coherence of the electron plays the dominant role in determining the transport characteristics, and the multi-subband scatterings tend to diminish such quantum effects.

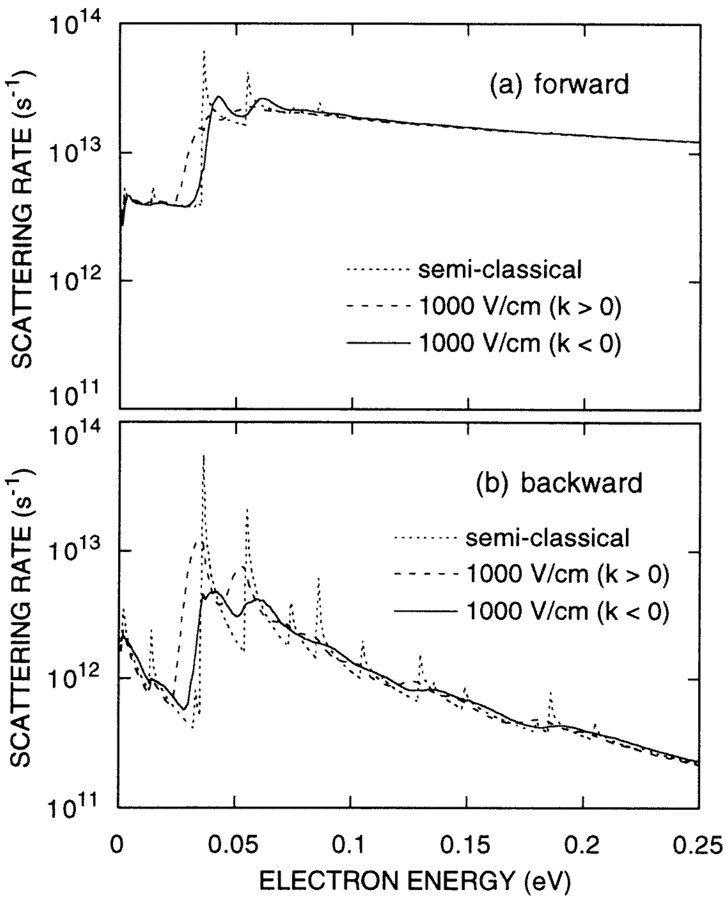

Figure 3. Rates of (a) forward and (b) backward scattering of confined LO phonons in the thick quantum wire ($L_y = 30$ nm and $L_z = 30$ nm) under $F = 1000$ V cm^{-1} and for $T = 300$ K. The dotted lines represent the rates obtained from Fermi's golden rule.

4. Summary

The rates of scattering of confined phonons in quasi-one-dimensional quantum wires have been evaluated by taking into account the ICFE. We have found that the ICFE makes the phonon scattering rates asymmetric with respect to the direction of the electron propagation and that this asymmetry is noticeable even when multi-subband scatterings are significant in thick quantum wires. Furthermore, the ICFE greatly modifies the strength and energy dependence of the backward scattering and, thus, it is expected that the electron-transport properties could be affected by the ICFE.

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