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Drift-velocity degradation caused by an electric field during collision in one-dimensional quantum wires

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Electron transport in quasi-one-dimensional quantum wires under high electric fields is investigated with the Monte Carlo method. The intracollisional field effect that is associated with the energy change of the electron due to the high electric field during the finite collision duration is taken into account. It is shown that the electron drift velocity, contrary to previous predictions made with semiclassical treatments, is greatly reduced under moderately strong electric fields ($\gtrsim$ hundreds of V/cm). This holds true even if the electron confinement is not strictly strong in thick quantum wires so that multisubband scatterings are involved in determining the electron transport properties. [S0163-1829(96)52536-1]

The low-dimensional structures made feasible by the recent technology of lithography and crystal growth have attracted much attention because of their possible applications to future semiconductor devices. In particular, quasi-one-dimensional structures have been expected to show much higher mobility compared with that in bulk since the momentum space of electrons is strongly restricted in one direction so that the ionized impurity scatterings might be greatly suppressed.[1] According to a series of theoretical studies, Leburton *et al.*[2] have shown that, owing to the dramatic change of the phonon scattering rates associated with the one-dimensional (1D) density of states, the electron drift velocity limited by optical phonons is indeed enhanced in 1D structures. On the other hand, recent Monte Carlo simulations in which intersubband scatterings are taken into account have revealed that the electron drift velocity is not actually enhanced at room temperature, but rather similar to that in bulk.[3] Therefore, inclusion of multisubband scatterings seems to be critical to determine the electron transport characteristics.

It should be noted, however, that these analyses are based on the semiclassical Boltzmann transport equation and any quantum effects inherent in such high-temperature electron transport are ignored. Very recently, we have pointed out that the intracollisional field effect (ICFE) that is associated with the energy change due to the external electric field during the collision duration with phonons might be important even under moderately strong electric fields in low-dimensional structures.[4] This is mainly due to the fact that the electron motion is restricted to the dimension parallel or antiparallel to the electric field so that the ICFE could be *always* significant in each scattering event with phonons. Notice that this is a marked contrast to the cases in bulk where there is no restriction on the direction of electron's motion.

In the present paper, we carry out the Monte Carlo simulations[5] of high-temperature electron transport in GaAs 1D quantum wires, taking into account both the ICFE and intersubband phonon scatterings. The present results demonstrate that the electron drift velocity is greatly reduced under moderately strong electric fields ($\gtrsim$ hundreds of V/cm) by the ICFE, and this holds true even if the electron confinement is not strictly strong in thick quantum wires so that multisubband scatterings are involved in determining the electron transport characteristics.

The quantum kinetic transport equation (the Barker-Ferry equation[6]) for the one-particle distribution function of electrons is our starting point. The Barker-Ferry equation could be derived from the quantum Liouville equation for the reduced electron density matrix.[7] In addition, we have assumed rectangular 1D quantum wires with an infinitely deep potential well in the transverse (y and z) directions. As a result, the electronic state is completely decoupled in the three different directions and the treatment of the Barker-Ferry equation is greatly simplified. Under the constant electric field $\mathbf{F}$, the Barker-Ferry equation for nondegenerate electrons is given by

$$\frac{\partial f_{\mathbf{k}}(t)}{\partial t} - e\mathbf{F}\cdot\frac{\partial f_{\mathbf{k}}(t)}{\partial \mathbf{k}} = 2\mathrm{Re}\sum_{\mathbf{q},\eta=\pm}\int_0^t d\tau |M_{\mathbf{q}}|^2 \left(N_{\mathbf{q}}+\frac{1}{2}+\frac{\eta}{2}\right) \times\{e^{-i(\varepsilon_{\mathbf{k}_F}+\eta\mathbf{q}-\varepsilon_{\mathbf{k}_F}-\eta\omega_{\mathbf{q}})\tau} f_{\mathbf{k}_F-\mathbf{q}}(t-\tau) - e^{-i(\varepsilon_{\mathbf{k}_F-\eta\mathbf{q}}-\varepsilon_{\mathbf{k}_F}+\eta\omega_{\mathbf{q}})\tau} f_{\mathbf{k}_F}(t-\tau)\}, \tag{1}$$

with $\mathbf{k}_F=\mathbf{k}-e\mathbf{F}\tau$. Here, $f_{\mathbf{k}}$ is the electron distribution function, $\varepsilon_{\mathbf{k}}$ is the electron energy with wave vector $\mathbf{k}$, $\mathbf{q}$ is the phonon wave vector, e is the magnitude of the electron charge, $M_{\mathbf{q}}$ is the matrix element for the Fröhlich electron-phonon interaction, $\omega_{\mathbf{q}}$ is the longitudinal-optical (LO) phonon energy ($=36$ meV for GaAs), and $N_{\mathbf{q}}$ is the phonon occupation number given by the Bose-Einstein statistics. $\eta=1(-1)$ for phonon emission (absorption). In the present study, we have considered only the confined Fröhlich LO-phonon scattering,[8] since the electron mobility under high electric fields ($\gtrsim$ hundreds of V/cm) is dominantly determined by LO phonons, and other scatterings such as acoustic phonons and surface-optical phonons could be safely ignored.[3] Also, we use the units of $\hbar=1$ throughout the paper.

The only difference between Eq. (1) and the semiclassical Boltzmann transport equation lies in the collision integral

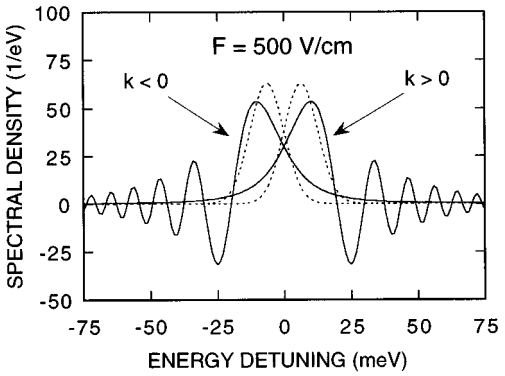

FIG. 1. Electron spectral densities as a function of energy detuning for the electron propagating to the positive ($k>0$) and negative ($k<0$) directions under $F=500$ V/cm (solid lines). The electric field is assumed to be directed to the negative direction. The dotted lines represent the approximated spectral densities employed in the Monte Carlo simulations.

[the right-hand side of Eq. (1)], i.e., the time retardation of the collision dynamics with phonons is included in Eq. (1). Because of this time retardation, numerical evaluation of Eq. (1) is still a formidable task. Ignoring the time retardation of the electron distribution function,[9] the collision integral I_c in Eq. (1) could be rewritten as

$$I_c=2\pi\sum_{\mathbf{q},\eta=\pm}|M_{\mathbf{q}}|^2\left(N_{\mathbf{q}}+\frac{1}{2}+\frac{\eta}{2}\right)\times\{S(\eta,\mathbf{q},\mathbf{k}_F)f_{\mathbf{k}-\mathbf{q}}(t)-S(-\eta,\mathbf{q},\mathbf{k}_F)f_{\mathbf{k}}(t)\},\quad(2)$$

where the spectral density $S(\eta,\mathbf{q},\mathbf{k}_F)$ is given by

$$S(\eta,\mathbf{q},\mathbf{k}_F)=\frac{1}{\pi}\int_0^\infty d\tau e^{-\Gamma_{\mathbf{k}}\tau}\cos[(\varepsilon_{\mathbf{k}_F+\eta\mathbf{q}}-\varepsilon_{\mathbf{k}_F}-\eta\omega_{\mathbf{q}})\tau].\quad(3)$$

$\Gamma_{\mathbf{k}}$ is the total LO-phonon scattering rate and we have here assumed that the time correlation between two successive scatterings is destroyed by a collision with phonon. Notice that when the electron lifetime is infinite ($\Gamma_{\mathbf{k}}=0$) and the electric field is suppressed ($F=0$), Eq. (3) correctly reduces to the energy-conserving δ function and Eq. (1) becomes identical to the semiclassical Boltzmann transport equation.

The spectral densities for phonon emission, evaluated by Eq. (3) for the electron moving parallel ($k<0$) or antiparallel ($k>0$) to the electric field of $F=$ 500 V/cm, are given in Fig. 1. The electric field is assumed to be directed to the negative direction. As already known,[10] the ICFE broadens the energy-conserving δ function and skews the energy detuning (zero point). Both effects are directly related to the strength and direction of the electric field, and the magnitude of both broadening and shift, Δ_F, is approximately given by $\Delta_F\sim[e|\mathbf{q}\cdot\mathbf{F}|/(2m')]^{1/2}$, where m^* is the electron effective mass. The most important feature here is that 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 ($k>0$), the spectral density shifts to the positive direction, and *vice versa*. Its physical

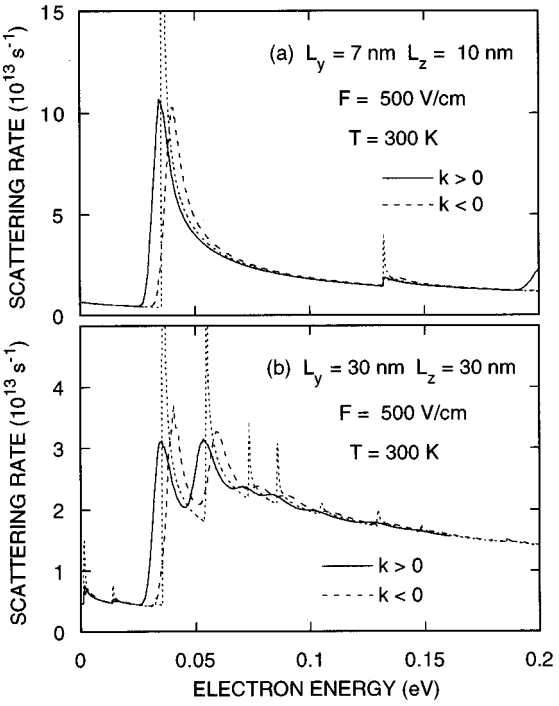

FIG. 2. Electron–LO-phonon scattering rates from the lowest subband to the first 20 subbands under $F=500$ V/cm for (a) 7 nm×10 nm and (b) 30 nm×30 nm quantum wires. The solid and dashed lines represent the scattering rates when the ICFE is taken into account and correspond to the rates for the electron with $k>0$ and $k<0$, respectively. The dotted lines show the semiclassical results obtained by Fermi's golden rule.

mechanism will be discussed along with the phonon scattering rates (Fig. 2) below. Since the electron motion is strictly confined along the electric field in 1D quantum wires, Δ_F is always finite and, thus, the ICFE is always effective. It should be noted that the ICFE is not always significant in 3D bulk because the phonon's wave vector $\mathbf{q}$ could be vanishingly small. Unfortunately, the spectral density shown in Fig. 1 is not positive definite. Therefore, we have approximated it by the Gaussian form in the following calculations, as done by Leburton *et al.*[2] when treating collisional broadening. The width and shift of the Gaussian spectral density are given by Δ_F. The approximated spectral densities employed here are also plotted by dotted lines in Fig. 1.

The confined Fröhlich LO-phonon scattering rates have been evaluated in terms of the Gaussian spectral density with $F=$ 500 V/cm at temperature $T=300$ K. Figure 2 shows the LO-phonon scattering rates from the lowest subband to the first 20 subbands for thin (7 nm ×10 nm) and thick (30 nm ×30 nm) quantum wires. Because of the energy broadening in the spectral density, the divergence of the scattering rate associated with the 1D density of states is removed (see the scattering rates from Fermi's golden rule indicated by dotted lines in Fig. 2). An interesting feature associated with the ICFE is, however, that the scattering rates become asymmetric with respect to the direction of the electron motion. This is closely related to the shift of the energy detuning in the spectral density, as seen in Fig. 1, and can be explained as follows. When an electron moves against the electric field ($k>0$), it gains energy from the electric field during the col-

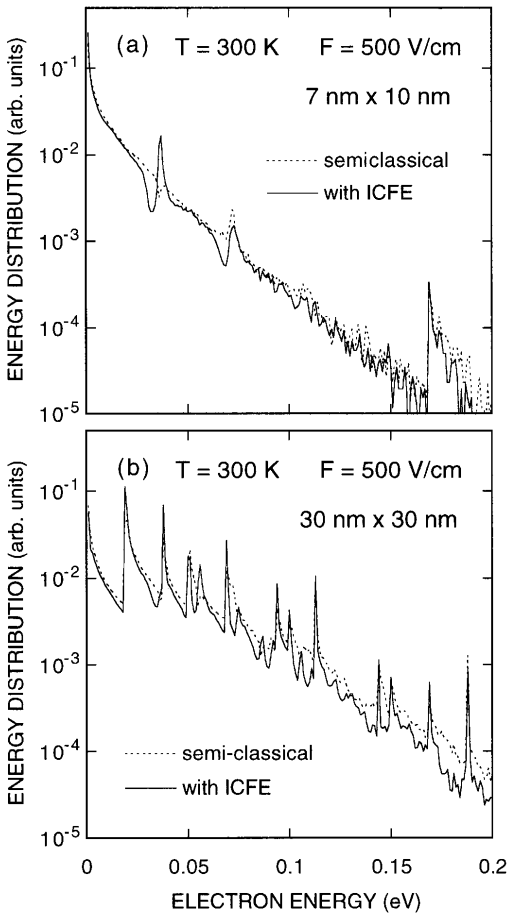

FIG. 3. Energy distribution functions as a function of electron energy for (a) 7 nm×10 nm and (b) 30 nm×30 nm quantum wires with $F=$ 500 V/cm and $T=$ 300 K. The solid lines represent the results when the ICFE is included in the Monte Carlo simulations, and the dotted lines are those obtained from the semiclassical Boltzmann transport equation. The electron energy is measured from the bottom of the lowest subband for each quantum wire.

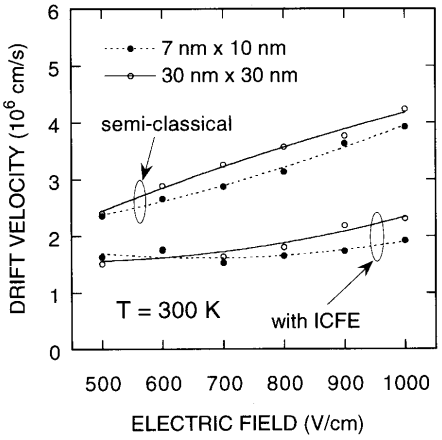

FIG. 4. Electron drift velocity as a function of electric field at $T=300$ K for 7 nm×10 nm (closed circles with dotted lines) and 30 nm×30 nm (open circles with solid lines) quantum wires. The drift velocities are reduced when the ICFE is included in both thin and thick quantum wires. The lines are only to guide the eye.

lision duration with 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 scattering rate shifts to the lower energy side. On the other hand, when it moves along the electric field ($k<0$), an electron loses its energy. Thus, the phonon energy is effectively increased and the scattering rate shifts to the higher energy side. Notice that this asymmetry is even more noticeable when the multisubband scatterings are significant in thick quantum wires [see Fig. 2(b)]. This is a direct consequence of the multipeak structure in the scattering rates associated with the intersubband scatterings. Therefore, the ICFE could be effective even if the size of 1D quantum wires are rather *large*.

The transport characteristics are determined from the Barker-Ferry equation given by Eq. (1). The conventional Monte Carlo method[5] has been applied to numerically solve it by substituting the Gaussian spectral density in the collision integral instead of the energy-conserving δ function.[11] The electron energy distribution functions thus obtained for thin and thick quantum wires are plotted in Fig. 3. Since the confinement is very strong in the present thin quantum wire (7 nm×10nm), the transport properties are essentially determined by the electrons in the lowest subband. As a result, the distribution function shows a multipeak structure with the phonon's energy, which results from the energy broadening by ICFE. This is consistent with the results when collisional broadening has been included by Leburton *et al.*[2] On the other hand, the peak structure associated with the phonon's energy disappears for a thick quantum wire (30 nm×30 nm) and the multipeak structure due to the intersubband scatterings becomes more apparent. In either quantum wire, however, the overall structures of the distribution functions become rather different between the quantum-mechanical (with the ICFE) and semiclassical results. Therefore, asymmetry in the phonon scattering rates modifies the occupancy of electrons in energy space.

Figure 4 shows the electric-field dependence of the electron drift velocity at room temperature for the two different quantum wires. The drift velocity evaluated by the semiclassical Boltzmann transport equation is also shown for comparison. We would like to stress that the drift velocity is greatly reduced when the ICFE is included and the reduction becomes greater as the electric field increases. This is because the scattering rate shifted to the lower-energy side for the electrons with ($k>0$), as a whole, determines the transport properties, since more electrons tend to occupy the positive wave-vector states (recall that the electric field is directed to the negative direction). In addition, it is interesting to note that the reduction of the drift velocity is relatively independent of the size of the quantum wire. Consequently, the drift velocity degradation is mainly ascribed to the asymmetric phonon scattering rates associated with the ICFE and this is true even for *thick* quantum wires.

In conclusion, electron transport under high electric fields in quasi-one-dimensional quantum wires has been investigated along with the intracollisional field effect. We have shown that the ICFE makes the phonon scattering rates asymmetric with respect to the direction of electron propa-

gation and, thus, already significant under moderately strong electric fields ($\gtrsim$ hundreds V/cm) in one-dimensional quantum wires. Employing the Monte Carlo method, we have demonstrated that the electron drift velocity is greatly reduced compared with that obtained via semiclassical treatments, and this holds true even when the multisubband scatterings have taken place in *thick* quantum wires.

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[9] This point is, of course, not at all trivial in low-dimensional structures; since electron transport is mainly controlled by the electrons with energy up to the LO-phonon energy, the spread in energy space of the electron distribution function is not quite large and the time retardation of the energy distribution might be important. The study on this point is under investigation and the results will be presented elsewhere.
[10] For example, see L. Reggiani, Physica **134B**, 123, (1985).
[11] The ICFE has been treated in a similar way for 3D electron gas in bulk materials by L. Reggiani, P. Lugli, and A.-P. Jauho [J. Appl. Phys. **64**, 3072 (1988)].