MONTE CARLO SIMULATION OF ELECTRON STREAMING CAUSED BY INELASTIC ACOUSTIC-PHONON SCATTERING IN QUANTUM WIRES

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Abstract

We have simulated by the Monte Carlo technique a ***qualitatively new*** regime of electron transport in quantum wires, which resembles electron streaming. Unlike conventional streaming caused by optical-phonon scattering, the streaming reported here is due to inelastic ***acoustic-phonon*** scattering. Both the analytical model and the Monte Carlo simulations yield $E^{1/5}$ field dependence of the drift velocity as a function of electric field E in the streaming regime. We demonstrate that this regime of electron transport is accompanied by strong radiation of nonequilibrium acoustic phonons from a quantum wire.

I. INTRODUCTION

Qualitatively new regime of electron transport in quasi-one-dimensional (1D) quantum wires (QWIs) has been predicted recently [1]. This regime resembles electron streaming and originates from strongly inelastic acoustic phonon scattering in QWIs [2]. Unlike conventional streaming due to electron scattering by optical phonons [3-5] the streaming-like electron behavior reported in [1] is caused by strongly inelastic acoustic-phonon scattering. The streaming due to acoustic-phonon emission leads to non-linear velocity-field dependence and to oscillating electron velocity autocorrelation function.

In this paper we present the results of Monte Carlo simulation of electron streaming due to acoustic-phonon emission in QWIs.

II. ANALYTICAL APPROACH

Let us first consider idealized model in order to obtain simple analytical expressions. We neglect acoustic-phonon absorption and assume that electrons are scattered exactly to the subband bottom after emission of acoustic phonon. Let us define ϵ_c as the characteristic acoustic-phonon energy determined by uncertainty of momentum conservation in 1D structures. It is given [2] by $\epsilon_c \approx 2\pi\hbar u/L$ where u is the sound velocity in the material of a QWI and L is the effective thickness of the structure $L^{-2} = L_y^{-2} + L_z^{-2}$. At low energies ($\epsilon < \epsilon_c$) the acoustic-phonon emission rate can be approximated by:

$$\lambda(\epsilon) = \Lambda\, \epsilon^2 \,, \tag{1}$$

where Λ is a constant independent of cross-section of a QWI. The mean free flight time $<\tau>$ generally reads as,

$$<\tau> = \int_0^\infty d\tau\; \tau\; \lambda[\epsilon(\tau)]\; \exp\left(-\int_0^\tau dt\; \lambda[\epsilon(t)]\right) \,, \tag{2}$$

where λ is the total scattering rate, in our case equal to acoustic-phonon emission rate given by Eq. (1). In electric field electron momentum during free flight is governed by: $dp/dt = eE$. Substituting energy expressed through momentum $\epsilon = p^2/2m^*$ and assuming that electron after a free flight is scattered exactly to the subband bottom, we get the solution in the form of $\epsilon = (eEt)^2/2m^*$. Substituting it into Eq. (1), then Eq. (1) into Eq. (3), and performing integration we get,

$$<\tau> = \left(\frac{5}{\Lambda C^4 E^4}\right)^{1/5} \Gamma \,, \tag{3}$$

where $\mathcal{C} = e/\sqrt{2m^*}$ and constant $\Gamma = \Gamma(6/5) \approx 0.9182$ is the value of the Gamma function. Then averaging energy $\epsilon(t)$ over the mean free flight $0 - <\tau>$ we find the mean electron energy,

$$<\epsilon> = \frac{\hbar\omega}{3}, \tag{4}$$

where $\hbar\omega$ is the average acoustic-phonon energy emitted by electrons,

$$\hbar\omega = \left(\frac{5\mathcal{C}}{\Lambda}\right)^{2/5} \Gamma^2 \, E^{2/5} \,. \tag{5}$$

Similarly averaging instant electron velocity over $<\tau>$ the drift velocity is obtained,

$$v_d = \sqrt{\frac{\hbar\omega}{2m^*}} \,. \tag{6}$$

Hence, the mean electron energy is a $E^{2/5}$ function and the drift velocity is $E^{1/5}$ function of the electric field. The drift velocity and the mean electron energy are simply related to each other: $<\epsilon>= 2/3\ m^*\ v_d^2$. The relationships (4) and (6) are the same as for conventional streaming due to optical phonon emission [5], but the characteristic acoustic phonon energy (5), unlike optical phonon energy, depends on electric field. Therefore, in contrast to conventional streaming where v_d and $<\epsilon>$ saturate [5], the streaming due to acoustic-phonon emission leads to field-dependent v_d and $<\epsilon>$.

The conventional streaming due to optical phonons can be realized if certain conditions are met [4]: (i) the temperature must be low enough, generally $k_BT \ll \hbar\omega$, where $\hbar\omega$ is phonon energy, (ii) the phonon emission rate must exceed all other scattering rates near the emission threshold, (iii) the electric field should be strong enough to accelerate electron up to the phonon emission threshold without scattering, but weak enough to avoid deep electron penetration beyond the emission threshold and thus to assure scattering by phonon emission down to the conduction band bottom.

In the case of electron streaming due to periodic *acoustic*-phonon emission the first two conditions, however, are generally fulfilled for acoustic-phonon scattering if $\epsilon_c \gg k_BT$. Let us estimate the range of electric fields $E_{min} \ll E < E_{max}$, where the streaming due to acoustic-phonon emission occurs. First, we define the "passive region" as the energy range where acoustic-phonon emission rate is less than absorption rate. By requiring that electron acceleration time through the "passive region" be much less than the absorption time, we get the lower field limit E_{min}. The condition $\hbar\omega < \epsilon_c$ sets the upper field limit of E_{max}. The lower field limit E_{min} weakly depends on the cross-section and is approximately equal to 1 V/cm. The upper limit is around 200 V/cm for $40 \times 40 Å^2$ QWI, 35 V/cm for $80 \times 80 Å^2$ QWI, and 4 V/cm for $250 \times 150 Å^2$.

III. MONTE CARLO SIMULATIONS

1. Model

We have carried out Monte Carlo simulations of electron transport in a wide range of electric fields. We have considered rectangular GaAs QWIs embedded in AlAs with infinitely deep potential well for electrons. We have chosen several different cross-sections of a QWI, from rather thick $250 \times 150 Å^2$ QWI, where separation between two lowest subbands is less that optical phonon energy, to unrealistically thin $40 \times 40 Å^2$ QWI, which represents the extreme limit. Simulations have been performed for low temperature $T = 4\ K$ and non-degenerate electron gas. Electron scattering by confined longitudinal optical (LO) phonons and localized interface (surface) SO phonons [6,7] as well as by bulk-like acoustic phonons [2] has been taken into account in our model. Our model incorporates as many subbands as there are actually occupied by electrons. Ionized impurities are assumed to be located sufficiently far from the QWI so that their influence on the electron motion inside the wire is negligible.

2. Results

Fig. 1 demonstrates drift velocity as a function of electric field calculated by the Monte Carlo technique. There are four distinguishable regions on velocity-field dependence. The near-ohmic velocity-field dependence in a field range below 1 V/cm turns into a sub-linear dependence. Then the slope again increases and decreases approaching saturation at high electric fields. The first sub-linear region extends through the two orders of magnitude in electric fields in $40 \times 40\text{Å}^2$ QWI (2 V/cm to 200 V/cm) and appears just as a small kink in $250 \times 150\text{Å}^2$ QWI at around 2 V/cm. In the field range of 5 V/cm to 200 V/cm in $40 \times 40\text{Å}^2$ electron drift velocity increases near as $E^{1/5}$ function of electric field as is predicted by Eqs. (5)–(6). Note that this field range coincides with the above estimated range $1\ \text{V/cm} \ll E < 200\ \text{V/cm}$ for this QWI, where electron streaming due to acoustic-phonon emission occurs. At high electric fields the optical-phonon emission starts dominating and the drift velocity saturates. The transition from the acoustic-phonon controlled electron transport to the optical-phonon controlled transport occurs at lower electric fields in thick QWIs, where acoustic phonon scattering rate is lower [2].

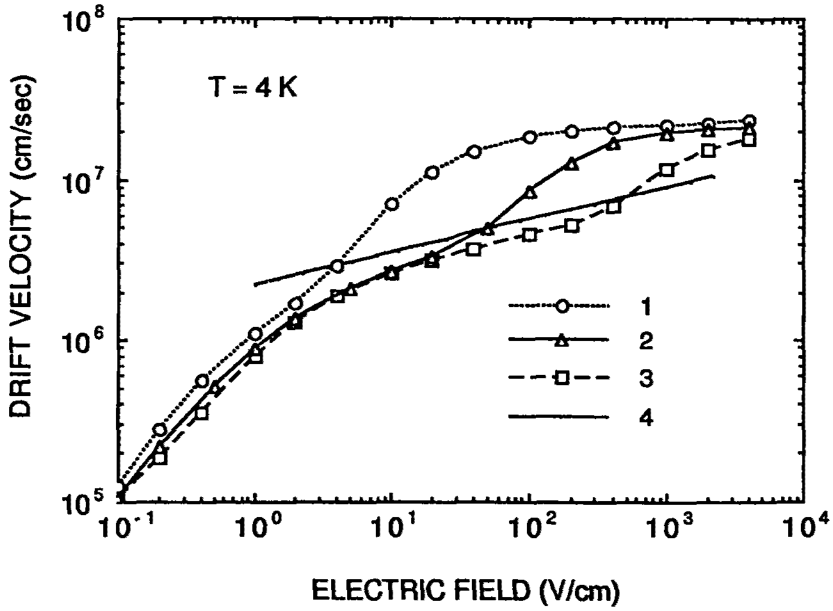

Fig. 1. Electron drift velocity versus applied electric field. Curve 1 represents velocity for $250 \times 150\text{Å}^2$ QWI, curve 2 – $80 \times 80\text{Å}^2$ QWI, and curve 3 – $40 \times 40\text{Å}^2$ QWI; curve 4 represents analytical dependence given by Eqs. (6) and (5).

Fig. 2 demonstrates the relative scattering efficiency (ratio of the number of corresponding scattering events to the total number of real scattering events) versus electric field. One can see that in the field range below about 1 V/cm there is a balance between acoustic-phonon absorption and emission efficiency indicating the ohmic regime of electron transport. Then the emission efficiency gradually increases and the absorption efficiency decreases up to electric fields of about 200 V/cm reflecting the transition to the acoustic phonon controlled electron streaming. The emission of acoustic phonons remains the sole scattering mechanism in the field range of 10 V/cm to 200 V/cm. Strong emission of acoustic phonons suggests that QWIs should radiate nonequilibrium acoustic phonons in the streaming regime. The question is which part of this radiation is directed along the QWI and which part goes into surrounding material. The ratio of the transverse component of acoustic phonon wave vector to the total magnitude of the wave vector $\eta = q_T/\sqrt{q_x^2 + q_T^2}$ roughly defines the relative fraction of the radiation going outside a QWI in the total radiation of acoustic phonons. We have calculated η as a function of electric field by the Monte Carlo technique. Our calculations show that $\eta \geq 0.98$ in the entire field range of 1 V/cm to 1000 V/cm. Consequently, a QWI radiates acoustic phonons predominantly in the perpendicular to a QWI direction. We believe that strong radiation of nonequilibrium acoustic phonons and their angular distribution could be experimentally measurable in the streaming regime.

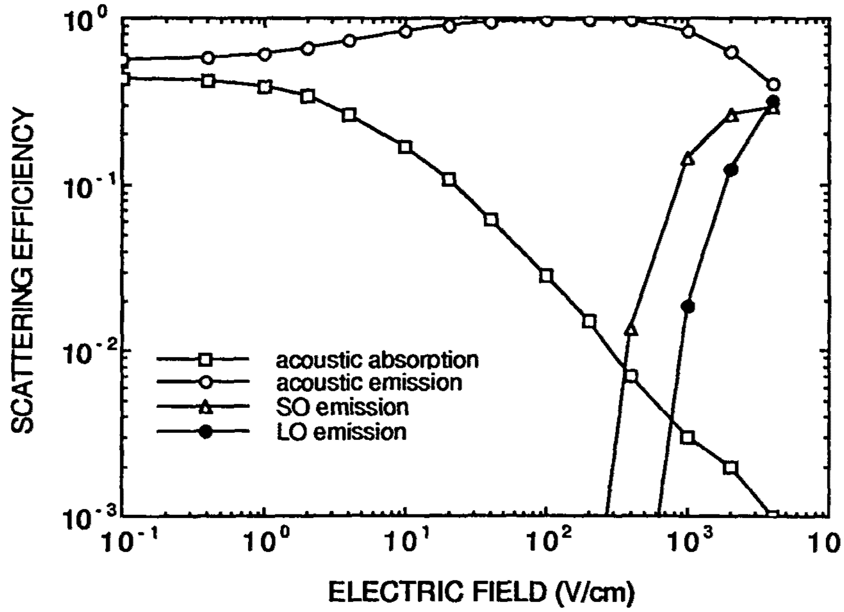

Fig. 6. Relative efficiency of various scattering mechanisms versus electric field for $40 \times 40 Å^2$ QWI.

The fields of about 300 V/cm and up are strong enough to heat the electrons up to the lowest optical phonon energy (in our case, GaAs-like interface mode energy equals 34.5 meV) and one can see the rapid onset of SO phonon scattering. With further increase of electric field the LO phonon scattering comes into play, and thus the electron transport in the fields exceeding 400 V/cm is primarily controlled by optical phonon scattering.

IV. SUMMARY

We have investigated qualitatively new regime of electron transport in QWIs, which closely resembles electron streaming due to *acoustic-phonon* emission. Both analytical and Monte Carlo calculations yield non-linear velocity-field relationships in the streaming regime. It is demonstrated that a QWI becomes effective radiator of nonequilibrium acoustic phonons in the streaming regime.

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