MONTE CARLO SIMULATION OF NONEQUILIBRIUM ELECTRON-PHONON SYSTEM IN QUANTUM WIRES

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Abstract

The ensemble Monte Carlo method for simulating relaxation of the nonequilibrium electron-phonon system in quasi-one-dimensional quantum wires is presented. Employing this method we have found that nonequilibrium (hot) phonon effects in quantum wires are well pronounced for electron concentrations higher than $10^5\ cm^{-1}$ and depend strongly on the energy distribution of excited electrons. Two opposite effects of nonequilibrium phonons in two different relaxation stages have been revealed. The buildup of hot phonons leads to the substantial reduction of the electron gas cooling rate for $t > 0.5\ ps$ due to strong reabsorption of nonequilibrium phonons. In contrast, the very initial relaxation stage ($t < 0.5\ ps$) is faster in the presence of hot phonons.

I. INTRODUCTION

When electrons are heated well above the lattice temperature they relax via cascade emission of phonons and drive the phonon system out of equilibrium. Hot phonons, in turn, affect the entire relaxation dynamics of hot electron gas. Moreover, the quasi-one-dimensional (1D) nature of electrons and optical phonons in quantum wires (QWIs) results in some specific peculiarities of hot phonon buildup that strongly modify nonequilibrium electron-phonon dynamics in QWIs [1]. Therefore, it is necessary to simulate coupled nonequilibrium electron-phonon system self-consistently [1,2].

In this paper we present ensemble Monte Carlo simulation results of the relaxation of 1D nonequilibrium electron-phonon system in QWIs after short pulse excitation. The accurate allowance for the peculiarities of coupled nonequilibrium 1D electron-phonon system within the Monte Carlo technique is discussed.

II. PECULIARITIES OF 1D ELECTRON-PHONON SYSTEM

In general, the phonon wave number is defined by the energy and momentum conservation equations and is given by:

$$q = \sqrt{k^2 + k'^2 - 2kk'\cos\theta}\ , \tag{1}$$

where k is the electron wave number before scattering, $k' = \sqrt{k^2 \pm 2m^*\omega_o/\hbar}$ is the electron wave number after absorption (sign +) or emission (sign −) of the optical phonon of frequency ω_o, and θ is the angle between electron wave vectors before and after scattering. Due to optical phonon quantization and the resultant 1D momentum conservation in quantum wires, electrons can emit or absorb optical phonons with wave vectors which are strictly defined by the electron momentum and the phonon energy. In 1D structures there are just two final states for scattered electrons: forward scattering with $\cos\theta = 1$ or backward scattering with $\cos\theta = -1$. Consequently, there are two possible phonon wave vectors available for emission (and two for absorption) by any single electron:

$$q_{min} = |k - k'|,\ \ q_{max} = k + k'. \tag{2}$$

In contrast, in quasi-two-dimensional (2D) quantum wells (or bulk materials) due to existence of additional degree(s) of freedom, $\cos\theta$ can take any value in the range $(-1, +1)$, so that there is an

entire range of a phonon q values from $|k - k'|$ to $k + k'$ available for electron interactions. Fig. 1 depicts q_{min} and q_{max} as a function of electron energy. The dashed area shows the region of available phonon modes for electron to interact with in bulk (3D) or 2D systems. In 1D systems electrons can emit optical phonons only with wave numbers represented by the curve surrounding this dashed area. It is evident from Fig. 1 that nonequilibrium phonon distributions generated by electrons with different energies in 2D and bulk systems overlap. In contrast, electrons in QWIs with different energies generate nonequilibrium phonons in different q-space points. Hence, unlike in 2D and 3D systems nonequilibrium phonons in QWIs can be reabsorbed only by the electrons that have generated them. Consequently, in bulk materials and quantum wells the reabsorption rate for any single electron generally depends on the total phonon population, whereas in QWIs it depends on the occupation number of just two modes with q_{min} and q_{max}. On the other hand, the total phonon population is proportional to the total electron concentration, while the occupation number of single modes is determined by the concentration of electrons with certain energies (*energetic density of electrons*). If the electron energy distribution spreads and the total concentration remains the same, the energetic density of electrons decreases. Therefore, the total nonequilibrium phonon population remains constant because more nonequilibrium phonon modes are amplified, but the occupation number of each mode decreases. As the result the reabsorption rate in 2D and 3D systems does not change with the spread of electron energy initial distribution (it depends on total phonon population), whereas the reabsorption rate in 1D systems decreases (it depends on particular phonon occupation numbers). We come to the fundamental conclusion that, *unlike in bulk materials and quantum wells, in QWIs hot phonon effects become more pronounced when narrowing energy distribution of excited (injected) hot electrons.*

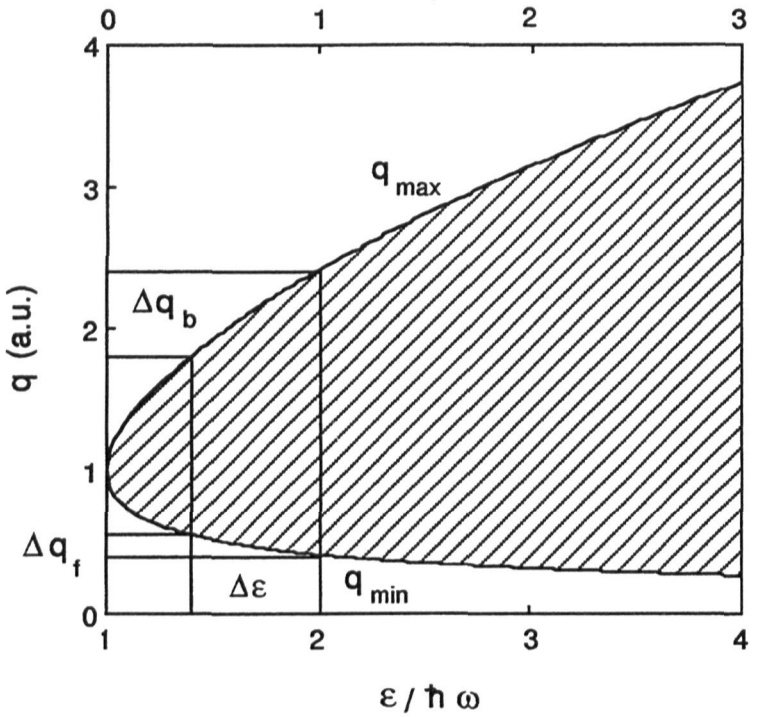

Fig. 1. Minimum and maximum phonon wave numbers versus electron energy normalized to phonon energy. The lower scale applies to emission and the upper for to absorption of phonons. Dashed area shows the range of phonon modes for electron scattering in 2D and 3D systems. The Δq_f and Δq_b depict the spread in nonequilibrium phonon distribution caused by electron energy spread $\Delta\epsilon$ for forward and backward scattering, respectively.

These peculiarities of hot phonon buildup in QWIs must be taken into account in numerical calculations. In Monte Carlo simulations of 3D and 2D nonequilibrium electron-optical phonon systems, the mesh interval for the phonon occupation number Δq is not a crucial parameter, provided that the interval is much less than the q-space region populated by nonequilibrium phonons: $\Delta q \ll q_{max} - q_{min}$. This region is sufficiently large (see Fig. 1) so that above condition is easily satisfied. However, in 1D systems, as we already mentioned above, there are just two single phonon

modes (q_{min} and q_{max}) available for a single electron to interact with. Therefore, when dealing with near-monoenergetic electron excitation virtually coherent phonon modes are amplified. Fig. 1 illustrates how energy broadening of excited electrons leads to the spread of phonon distribution in q-space. One can see that even substantial electron energy broadening ($\Delta\epsilon > \hbar\omega/2$) results in very narrow q-space region for hot phonons generated in forward scattering, Δq_f. Therefore, we generally cannot satisfy the condition $\Delta q \ll \Delta q_{f,b}$ because the fundamental limit of accuracy of determination of phonon wave vector sets the lower limit $\Delta q \geq 2\pi/L_x$, where L_x is the length of a QWI. For a QWI of the length $L_x = 10$ microns this limit is $2\pi/L_x \approx 6 \times 10^3\ cm^{-1}$.

III. MODEL AND METHOD

In our simulations we consider rectangular GaAs QWI embedded in AlAs. We have assumed infinitely-deep potential well for electrons. The hot electron energy dissipation model includes electron interactions with confined longitudinal optical (LO), localized surface (interface) optical (SO) phonons, and inelastic interaction with bulk-like acoustic phonons. We start the simulation of electron relaxation after the initial excitation by a short pulse with a duration of 0.1 ps. We have not simulated electron relaxation in coherent regime ($t < 100\ fs$) which requires a quantum mechanical description. Instead, we have focused our attention on the time range $t > 0.1\ ps$ when electrons can be treated semiclassically [3-6]. We do not take into account the electron-hole interaction. The initial state of electron relaxation accounts for the broadening of the electron energy distribution due to two effects: (i) uncertainty in electron initial energy due to the short electron lifetime at the excited level and (ii) spectral broadening of the exciting pulse with duration of the order of 0.1 ps [7]. In accounting for these effects we assume that they both lead to a Gaussian distribution of electron energy at $t = t_0$ [8], which corresponds to the end of the excitation pulse. We vary the excitation energy ϵ_{ex}, which corresponds to the center of a Gaussian distribution, as well as, $\Delta\epsilon$, the half-width of this distribution.

Hot phonon thermalization due to the decay of optical phonons into acoustic phonons is taken into account by recalculating N_q for every mesh interval at the end of each time step. For simulations we have used the bulk value of the phonon thermalization time $\tau_{ph} = 7\ ps$. We have not taken into account the increase in the acoustic phonon population as a result of the decay of nonequilibrium optical phonons. The reason for this is that acoustic phonons in a QWI embedded in surrounding material with similar elastic properties (GaAs in AlAs in our case) can easily penetrate through GaAs/AlAs interfaces and escape from the QWI. Therefore, we have excellent thermal conductivity and the QWI should not be heated much more than the whole GaAs/AlAs structure. Given that the surrounding AlAs is sufficiently massive, the increase in temperature would be negligible even if the QWI strongly radiates acoustic phonons.

IV. MONTE CARLO SIMULATION RESULTS

We have found that hot phonon effects in QWIs are well pronounced for electron concentrations of the order of $10^5\ cm^{-1}$ and depend strongly on the energy distribution of excited electrons. We have considered various half-widths of Gaussian electron distribution ranging from the extremelly narrow of 4 meV to the broad but still less than optical phonon energy of 30 meV. Figure 2 illustrates electron cooling dynamics in a $150 \times 250 \AA^2$ QWI at $T = 30\ K$ after initial electron excitation at an energy 4.5 times the LO phonon energy for two extreme limits of Gaussian electron distribution half-widths. For comparison, we plot the electron relaxation dynamics without nonequilibrium optical phonons. One can see that hot phonons lead to a substantial reduction of the electron gas cooling rate for $t > 0.5\ ps$ due to strong reabsorption of nonequilibrium phonons [1]. In contrast, the very initial relaxation stage ($t < 0.5\ ps$) is faster in the presence of hot phonons. As we have already mentioned above, hot phonon effects in both relaxation stages are more pronounced for narrow electron distributions (see Fig. 2). Hence, the higher nonequilibrium phonon populations are created (4 meV), the faster is the very initial relaxation stage.

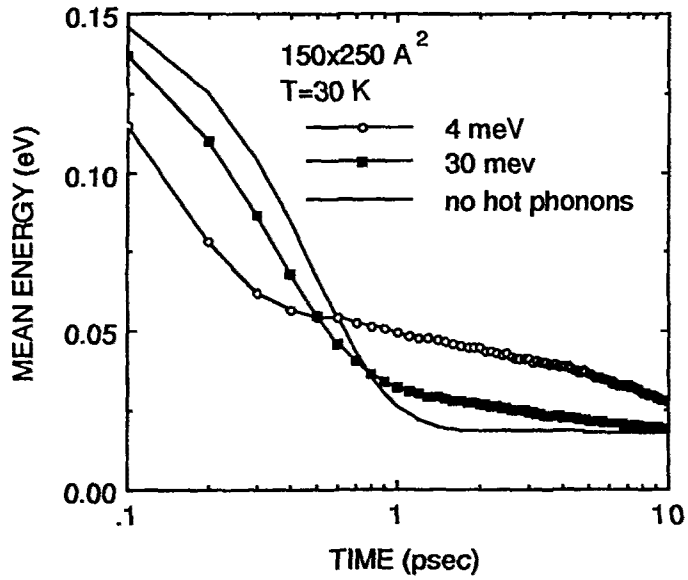

Fig. 2. Mean electron energy as a function of time after initial electron excitation at an energy equal to 4.5 times the LO phonon energy, for two initial widths of electron energy distribution. Electron concentration is $n = 10^5 cm^{-1}$ and lattice temperature is $T = 30\ K$. Solid curve describes the energy evolution for the case of an equilibrium phonon distribution. Results apply to the case of a single-subband QWI neglecting SO phonons.

This effect can be understood if one first considers the temperature dependence of the relaxation rate. At high temperatures both the emission and absorption rates are higher. This leads to fast energy redistribution of excited electrons. The cooling rate of electrons which emit optical phonons increases and that of electrons which absorb phonons decreases because of the $\epsilon^{-1/2}$ energy dependence of 1D density of states and scattering rates. The increase, however, is faster than the decrease due to the same $\epsilon^{-1/2}$ function. Therefore, the total 1D electron gas cooling rate increases when the electron energy redistributes due to emission and absorption of optical phonons. Hence, the very initial electron cooling rate in QWIs increases when increasing the lattice temperature, provided that electrons are excited well above optical phonon energy and thermal equilibrium energy. To observe an appreciable temperature effect on the relaxation rate it is necessary that phonon occupation number be greater than 1. Under phonon equilibrium such occupation numbers could even be unachievable in a solid state. However, due to strong buildup of nonequilibrium phonons at high excited electron concentrations the occupation number for certain phonon modes may be considerably higher than 1. This is why the initial relaxation is faster for higher nonequilibrium phonon occupations and thus, for narrower initial electron energy distributions.

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