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Hot phonons in quantum wires

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Abstract. We present results of Monte Carlo simulations of electron relaxation dynamics in rectangular GaAs quantum wires (QWIS) embedded in AlAs. Electron interactions with confined LO phonons, interface optical phonons, bulk-like acoustic phonons as well as non-equilibrium (hot) optical phonons have been taken into account. It has been found that hot phonons come into play at electron concentrations exceeding 10^5 cm^{-1}. In QWIS electrons having appreciably different initial energies generate non-equilibrium phonons at different q-space regions which do not overlap. In turn, these phonons can be reabsorbed only by the electrons that have generated them. Consequently, hot-phonon effects become weaker as the energy distribution of excited electrons broadens. This result is in complete contrast to the case of bulk materials and quantum wells where the injected electron energy distribution virtually does not affect non-equilibrium phonon build-up and the reabsorption rate.

In virtually all microelectronic and optoelectronic devices electrons are heated considerably above the lattice temperature. Hot electrons relax via cascade emission of phonons and drive the phonon system out of equilibrium. It is now a commonly accepted notion that non-equilibrium (hot) phonons strongly affect electron transport and relaxation in bulk materials [1, 2]. Hot-phonon effects also explain observations of very slow electron cooling in quantum wells following subpicosecond photoexcitation of hot electrons [3]. For the same reasons, hot electrons should induce hot phonons in the quasi-one-dimensional (1D) quantum wire structures which are currently attracting considerable scientific attention. Although non-equilibrium carrier dynamics in QWIS has been extensively studied (see, for example, [4, 5]), the hot-phonon problem has been addressed only recently [6, 7]. However, the approaches used in [6, 7] overlook some important peculiarities of hot phonons in 1D structures.

Owing to optical phonon quantization and the resultant 1D momentum conservation in quantum wires, electrons can emit or absorb optical phonons with wavevectors which are strictly defined by the electron momentum and the phonon energy. In general, the phonon wavenumber is defined by the energy and momentum conservation equations and is given by

$$q = \sqrt{k^2 + k'^2 - 2kk' \cos\theta} \qquad (1)$$

where k is the electron wavenumber before scattering, $k' = \sqrt{k^2 \pm 2m^*\omega_o/\hbar}$ is the electron wavenumber after absorption (sign +) or emission (sign −) of the optical phonon of frequency ω_o, and θ is the angle between electron wavevectors before and after scattering. 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 wavevectors available for emission (and two for absorption) by any single electron: $q_1 = |k - k'|$ and $q_2 = k + k'$. In contrast, in quantum wells (or bulk materials), owing to the 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 q from $|k - k'|$ to $k + k'$ available for electron interactions.

Therefore, electrons in QWIS having appreciably different energies generate non-equilibrium phonons in different q-space regions which do not overlap. In turn, these phonons can be reabsorbed only by the electrons that have generated them, unlike in bulk materials and in quantum wells where electrons can reabsorb phonons emitted by other electrons. Consequently, electrons which have different energies cannot interact through the emission and subsequent reabsorption of optical phonons. Thus, electrons and the phonons associated with them (with appropriate wavevectors) are isolated from other electron–phonon pairs if electrons are in different states. Only electrons in the same state can interact via the emission and subsequent reabsorption of optical phonons. However, since such electrons are indistinguishable, this interaction is physically meaningless. Thus, for 1D structures we must eliminate one cross-correlation effect which is always present in the non-equilibrium electron–phonon system in bulk materials and in quantum wells and which is important when considering electric noise [8].

Another consequence of the 1D nature of the electron–phonon interaction in QWIS is that the re-

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absorption probability for each single electron in the QWI does not depend on the integrated phonon occupation number but only on the occupancy at certain q. This reabsorption probability decreases as the phonon occupancy spreads over q-space (given that the integrated occupancy remains constant). The spread of the non-equilibrium phonon population in q-space results from the broadening of the electron energy distribution. As a result, the reabsorption rate and hot-phonon effects should depend strongly on the energy distribution of injected electrons.

We have performed Monte Carlo simulations of hot-electron relaxation in rectangular GaAs/AlAs quantum wires with a multisubband structure. Electron interactions with confined longitudinal optical (LO), surface (interface) optical (SO) phonons [9] and bulk-like acoustic phonons [10] as well as non-equilibrium optical phonon populations are taken into account. In accordance with the 1D nature of optical phonons in QWIS, the increment of phonon occupation number after each emission (sign +) or absorption (sign −) event is given by the term $(\pm 2\pi/\Delta q)(n/N)$, where Δq is the step of the mesh in q space used to collect the N_q histogram, n is the electron concentration per unit length of a QWI and N is the actual number of particles in the simulation.

In Monte Carlo simulations of bulk and 2D non-equilibrium electron–optical phonon systems, the step of the mesh Δq is not a crucial parameter, given that the step is much less than the q-space region populated by non-equilibrium phonons which can be estimated easily. This is due to the fact that the phonon reabsorption rate depends on the integrated (average) occupancy over the entire region which is not crucially sensitive to the step of mesh. However, in 1D systems, as we have already discussed, the reabsorption rate depends only on the local value of phonon occupancy, N_q, at an appropriate q value. Therefore, as the step becomes smaller, both the local occupancy and the reabsorption rate become larger. This problem is particularly important when considering near-monoenergetic electron injection (excitation). If one chooses too large a step the peculiarities related to the 1D nature of the electron–phonon system may be considerably washed out. There are, of course, physical limits on the magnitude of Δq. These limits follow from the uncertainty in the phonon wavenumber due to the finit length of the QWI. We have taken a QWI of length $L_x = 10\ \mu\text{m}$, so that $\Delta q = 2\pi/L_x \approx 6 \times 10^3\ \text{cm}^{-1}$.

Hot-phonon thermalization due to the decay of optical phonons into acoustic phonons is taken into account by recalculating N_q at the end of every time step. It has been demonstrated [11] that the phonon thermalization time, τ_{ph}, in low-dimensional structures depends weakly on the size of the structure and is close to the bulk value. For simulations at $T = 30$ K and 77 K, we have used the value $\tau_{ph} = 7$ ps [1]. The time step in our simulations has been chosen to be smaller than the average free-flight time and much less than the phonon thermalization time, τ_{ph}. We have not taken into account the increase in the acoustic phonon population as a result of the decay of non-equilibrium optical phonons. There are two reasons for this. First, the build-up of non-equilibrium optical phonons occurs only in a very narrow region of the Brillouin zone (near the centre), so that over the entire zone the average occupation number increases only negligibly. This is true for systems of any dimensionality since the electrons interacting with phonons populate only the centre region of the Brillouin zone. Second, the acoustic phonons in QWIS embedded in surrounding materials with similar elastic properties (GaAs in AlAs in our case) are bulk-like and they 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 will be negligible even if the QWI strongly radiates acoustic phonons.

Let us first consider a simplified picture in which there is only one energy subband and SO phonons are neglected; that is, only LO and acoustic phonons are present in the QWI. This simplified picture allows us to model the pure 1D effect of the broadening of the electron energy distribution on the build-up of hot phonons and on electron cooling dynamics. Figure 1 illustrates electron cooling dynamics in a $150 \times 250\ \text{Å}^2$ QWI at $T = 30$ K following initial electron excitation at an energy 4.5 times the LO phonon energy for two different Gaussian electron distribution halfwidths: 30 meV and 4 meV. The lower value of 4 meV excitation linewidth corresponds to the case of a near-perfect QWI where broadening of the energy levels due to variable cross section [9] can be neglected. For comparison, we plot the electron relaxation dynamics without non-equilibrium optical phonons. When hot phonons are neglected the cooling dynamics display two distinguishable stages: the fast stage (with subpicosecond duration) due to the cascade emission of optical phonons, and the second, slow stage of electron thermalization due to interactions with acoustic phonons. It must be noted, however, that in the time-scale of 10 ps acoustic phonon scattering does not visibly influence the electron relaxation dynamics in this QWI with a rather large cross section of $150 \times 250\ \text{Å}^2$. The electron concentration is chosen as $10^5\ \text{cm}^{-1}$ in figure 1(*a*) and as $10^6\ \text{cm}^{-1}$ in figure 1(*b*). As one can see from figure 1 the initial relaxation stage is faster in the presence of hot phonons. The higher the non-equilibrium phonon populations created (4 meV), the faster is the initial relaxation stage. This effect can be understood if one first considers the temperature dependence of the relaxation rate. At higher temperatures the initial electron distribution is rapidly broadened due to the stimulated emission and absorption of optical phonons. This happens on a time-scale where electron distribution at low temperatures may be still considered as unchanged. It is easy to show that due to increase in the difference between emission and absorption rates at lower energies in 1D systems the relaxation rate increases as the electron distribution broadens, provided that all electrons are still well above the optical phonon energy and thermal equilibrium energy. Consequently, at high temperatures the initial relaxation rate in QWIS is higher.

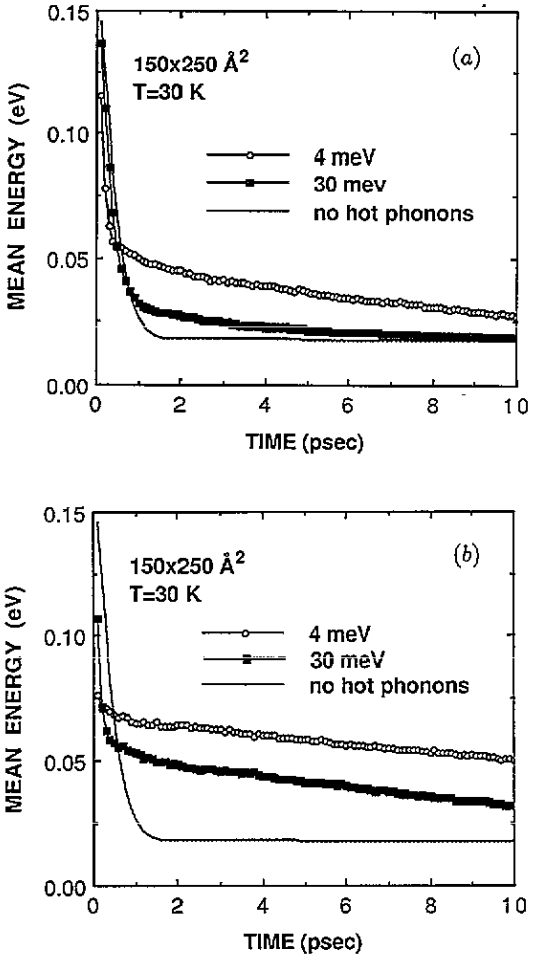

Figure 1. Mean electron energy as a function of time following initial electron excitation at an energy equal to 4.5 times the LO phonon energy, for two initial widths of the electron energy distribution. In both cases $T = 30$ K and the QWI cross section is 150×250 Å^2: (*a*) electron concentration $n = 10^5$ cm^{-1} and (*b*) $n = 10^6$ cm^{-1}. Full curves describe the energy evolution for the case of an equilibrium phonon distribution. Results apply to the case of a single-subband QWI neglecting SO phonons.

(Note that in bulk materials, where the difference between emission and absorption rates decreases with decreasing electron energy, the temperature effect is opposite: the relaxation rate is higher at low lattice temperatures. There should be no temperature dependence of the initial relaxation rate in 2D systems.) To observe an appreciable temperature effect on the relaxation rate it is necessary that the equilibrium phonon occupation number be much greater than 1, i.e. this effect manifests itself only at temperatures close to the melting point. However, a similar effect due to strong build-up of non-equilibrium phonons is easily observed (see figure 1) since the non-equilibrium phonon population may reach values as high as $\gtrsim 10$ for 10^6 cm^{-1} at certain very narrow regions of q-space.

The onset of the second relaxation stage, which is defined by the non-equilibrium phonon thermalization time, occurs sooner if the electron energy distribution is narrower (4 meV), i.e. for stronger build-up of non-equilibrium phonons. Hence, electron cooling is slower for narrow electron distributions. The effect of narrowing of electron energy distribution is similar to that of increasing the electron concentration and, as we have already discussed, it is a purely 1D effect.

It has been demonstrated [10] that in QWIS with small cross sections (40×40 Å^2) the acoustic phonon scattering rate is higher, and this scattering is much more inelastic than in QWIS with a large cross section (150×250 Å^2). Therefore, in a QWI with a 40×40 Å^2 cross section, acoustic phonon scattering is a very effective energy dissipation mechanism [12] and it is responsible for fast broadening of the electron energy distribution and, consequently, for smearing out the effect of the initial broadening of the electron distribution on the cooling rate. The role of acoustic phonons is discussed in much more detail in [12].

We have also considered the realistic case where the multisubband structure of the QWI is taken into account along with all possible optical phonon modes (LO and SO). Figure 2 shows the electron cooling dynamics in this realistic structure for 4 meV and 30 meV electron excitation linewidths. Note that the mean electron energy in this case is counted from the bottom of the lowest conduction subband and consists of the electron 'kinetic' energy of free 1D motion and 'potential' energy related to confinement, i.e. intersubband separation energy. The dependence of hot-phonon build-up on the electron distribution broadening is washed out considerably in this realistic structure due to various intrasubband and intersubband transitions assisted by the LO and the two SO modes. Indeed, non-equilibrium phonon peaks in q-space in this case overlap and form a complex broad distribution in q-space virtually independent of the initial electron distribution. The main effect which comes into play within this realistic model is the dependence of the number of the upper subbands involved in electron cooling on the initial electron energy distribution. Figure 3 demonstrates the time evolution of subband filling by electrons. In the case of broad electron initial distribution

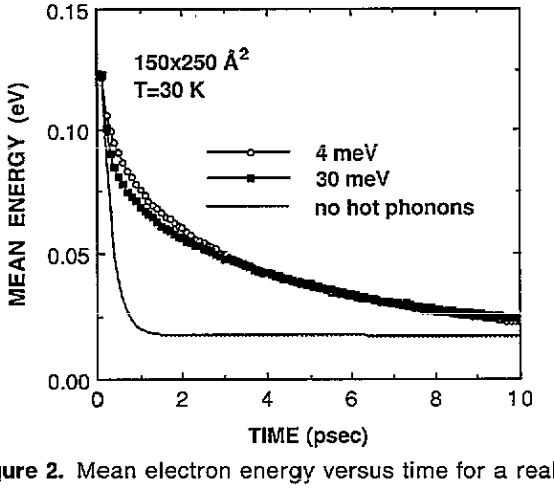

Figure 2. Mean electron energy versus time for a realistic multisubband QWI structure with both LO and SO optical modes and acoustic phonons included. Electron concentration is equal to $n = 10^6$ cm^{-1}; other parameters and conditions are the same as in figure 1.

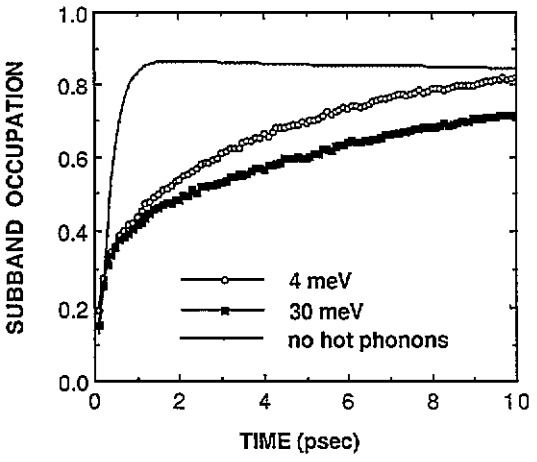

Figure 3. Time evolution of the relative occupation of the lowest subband. The parameters and conditions are the same as in figure 2.

(30 meV) there are more subbands occupied by electrons scattered from the high-energy tail. Therefore, the return of electrons to the first subband is slower than for a narrow electron distribution (4 meV). Hot phonons lead to the stronger intersubband electron redistribution and a slower return to the lowest subband (see figure 3). By comparing figures 2 and 3 one notices that the different occupation of subbands for 4 meV and 30 meV excitation linewidths virtually does not affect the mean electron energy, which coincides after 3 ps. This apparently strange behaviour is related to the fact that electron 'kinetic' energy related to 1D free motion in each subband is higher for 4 meV excitation linewidth owing to hot-phonon effects. This difference in kinetic energies is compensated by the higher occupation of the upper subbands in the case of 30 meV linewidth. Consequently, the 4 meV curve in figure 2 contains a larger part of 'kinetic' energy and a smaller part of 'potential' energy than the 30 meV curve.

In summary, we have investigated non-equilibrium electron–phonon dynamics in 1D quantum wire structures. We have employed the ensemble Monte Carlo technique which allows one to consider the electron–phonon system self-consistently. We have found that hot-phonon effects in QWIS are well pronounced for electron concentrations equal to or higher than 10^5 cm^{-1}. Hot-phonon effects become weaker as the broadening of the excited electron energy distribution increases. This result is in complete contrast to the case of bulk materials and quantum wells where the injected electron energy distribution virtually does not affect the build-up of non-equilibrium phonons and the reabsorption rate.

Acknowledgment

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