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Hot-electron overcooling and intersubband population inversion in quantum wires

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Abstract. Monte Carlo simulation of hot photoexcited electron relaxation in rectangular quantum wires is carried out. Simulation shows that at the initial stage the electron cooling dynamics is defined by electron–optical phonon interaction and exhibits strong dependence on excitation energy. When electrons are excited above the optical phonon energy they cool down in a subpicosecond time-scale to the bottom of the first subband. Electrons may even occur below thermal equilibrium energy and then slowly (during tens of picoseconds) relax to equilibrium due to interaction with acoustic phonons. At certain excitation energies strong intersubband electron scattering by optical phonons leads to carrier redistribution and intersubband population inversion.

Low-dimensional semiconductor structures are widely recognized as a very promising basis for optoelectronic applications. Lasers based on quantum wells are being successfully employed in industry because of their low manufacturing costs and obvious advantages with respect to conventional p–n junction lasers. Quasi-one-dimensional (1D) quantum wires (QWIs) are even more promising, and are expected to ensure better spectral characteristics, light coherence and differential gain owing to their unique peak-like density of states. Moreover, low dimensionality significantly reduces the threshold current and increases the efficiency of lasing. Extension of the modulation frequency band is also expected. In spite of this increasing interest in optoelectronic applications of 1D structures there are considerable gaps in the understanding of electron behaviour under realistic conditions where finite temperature, multisubband energy structure, external excitations and electron scattering must be taken into account. In order to design prospective optoelectronic devices based on 1D structures it is necessary to get a complete qualitative picture of electron dynamics under non-equilibrium conditions as well as quantitative estimates of various characteristics such as energy dissipation rates, momentum relaxation rates, recombination rates etc. Although there exist a number of publications dealing with relaxation processes in a 1D electron gas under quasistationary conditions (see, for example, [1, 2]), the relaxation dynamics of photoexcited non-equilibrium carriers has had little attention.

The goal of this paper is to present our recent results on Monte Carlo simulation of hot-electron relaxation dynamics in rectangular GaAs QWIs embedded in AlAs. Here, a two-dimensional infinitely deep square quantum well potential confines electrons in the QWI with a multisubband energy structure. We consider a non-degenerate electron gas with an electron concentration of the order of 10^5 cm^{-1} or less. The model includes hot-electron interactions with confined longitudinal optical (LO) and surface (interface) optical (SO) phonons [3–5] as well as essentially inelastic electron scattering by bulk-like acoustic phonons [6]. Since we are dealing with low electron concentrations non-equilibrium phonon effects are not included in our model (for non-equilibrium phonon effects in QWIs see [7]).

The initial state for electron relaxation accounts for electron energy distribution broadening due to two effects:

(i) uncertainty in the electron initial energy owing to the short electron average lifetime at the excited level ($\Delta\varepsilon \approx 10^{-2}$ eV for $\Delta t \approx 10^{-13}$ s);

(ii) spectral broadening of the exciting pulse with duration of the order of 10^{-13} s.

In accounting for these effects we assume that both lead to a Gaussian distribution of electron energy at $t = t_0$, which corresponds to the end of the excitation pulse. We vary the excitation energy ε_{ex}, which corresponds to the centre of the Gaussian distribution and a half-width $\Delta\varepsilon$ of this distribution. The results presented here correspond to $\Delta\varepsilon = 10$ meV. The initial electron distribution among subbands is considered to be defined by density of states for a given excitation energy in each subband.

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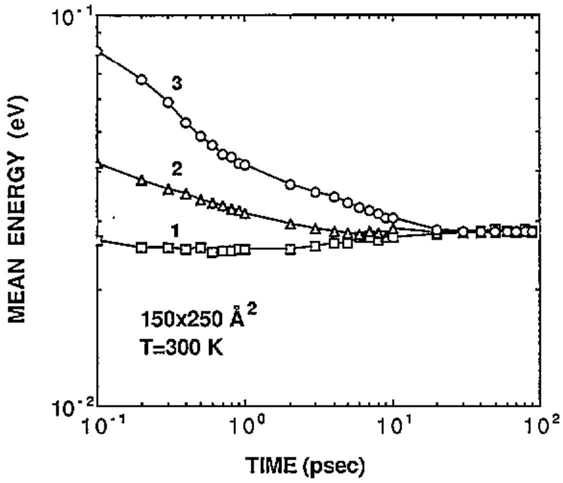

Figure 1. Time evolution of the mean electron energy in a QWI with a cross section of 150 × 250 Å^2 following excitation at a lattice temperature $T = 300$ K. Curve 1 corresponds to an excitation energy $\varepsilon_{ex} = 42$ meV, curve 2 to 67 meV, curve 3 to 100 meV. Subband energy positions in the QWI are counted from the bottom of the first (lowest) subband: 1st, 0 meV; 2nd, 28.5 meV; 3rd, 76 meV; 4th, 79 meV; 5th, 108 meV. $\hbar\omega_{LO} = 36.1$ meV.

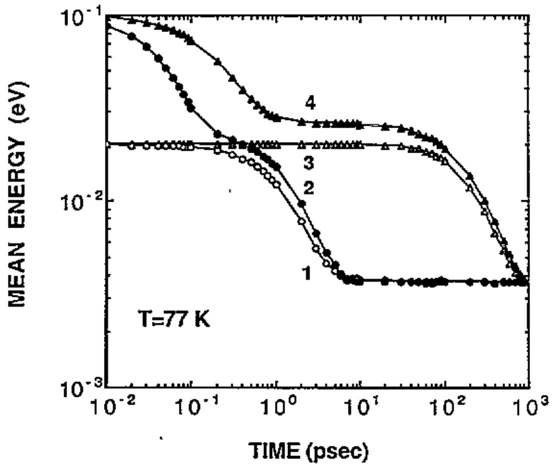

Figure 2. Time evolution of mean electron energy following excitation for QWIs with two different cross sections: 40 × 40 Å^2 (curves 1 and 2) and 150 × 250 Å^2 (curves 3 and 4). Curves 1 and 3 correspond to an excitation energy $\varepsilon_{ex} = 20$ meV, curves 2 and 4 to 100 meV. The second subband position in the QWI with a cross section of 40 × 40 Å^2 is counted from the bottom of the first subband and equals 105.5 meV. The lattice temperature is $T = 77$ K. $\hbar\omega_{LO} = 36.5$ meV.

Calculations with various excitation energies show that in the time-scale of 10^{-9} s electron relaxation exhibits two distinguishable stages. Figure 1 illustrates the electron cooling dynamics in a QWI with a cross section 150 × 250 Å^2 for different electron excitation energies ε_{ex} counted from the bottom of the lowest conduction subband. The first, or 'fast', stage in the mean electron energy dependence on time is observed when electrons are excited above the optical phonon energy ($\hbar\omega_{LO}$ or $\hbar\omega_{SO}$, where $\hbar\omega_{LO}$ and $\hbar\omega_{SO}$ are energies of LO and SO phonons respectively). As one can see from curve 3 corresponding to $\varepsilon_{ex} = 100$ meV, electrons initially (in the subpicosecond time-scale) cool down, losing their energy through interaction with optical phonons with the characteristic times $\tau_{e\text{-}LO} \approx 10^{-13}$ s and $\tau_{e\text{-}SO} \approx 10^{-12}$ s (for electron–LO phonon and electron–SO phonon interaction respectively). The duration of the 'fast' relaxation stage as well as the entire electron cooling dynamics during the 'fast' stage exhibits a strong dependence on the excitation energy. For excitation energy $\varepsilon_{ex} = 42$ meV we observe anomalous cooling dynamics when electrons occur below the thermal equilibrium energy, i.e. the electron gas becomes overcooled (curve 1 in figure 1). Electron gas overcooling occurs if the electron excitation energy falls into the range $\hbar\omega_{LO} < \varepsilon_{ex} < \hbar\omega_{LO} + k_B T/2$, where $k_B T/2$ is the electron equilibrium kinetic energy at a given temperature T corresponding to one degree of freedom in a QWI. At lower temperatures ($T = 77$ K) the transient electron overcooling disappears because the chosen broadening of electron initial energy distribution exceeds the electron thermal equilibrium energy $k_B T/2$.

The 'slow' stage of electron relaxation is controlled by the electron interaction with acoustic phonons. Our calculations demonstrate that at a lattice temperature $T = 300$ K the electron gas thermalization process in a QWI with a cross section of 150 × 250 Å^2 lasts about 30 ps (figure 1). This time strongly depends on the lattice temperature and on the cross section of the QWI, as does the acoustic phonon scattering rate [6]. Figure 2 demonstrates the electron cooling dynamics in a QWI with a cross section of 40 × 40 Å^2 compared with the cooling dynamics in a 150 × 250 Å^2 QWI. The electron energy relaxation due to interaction with acoustic phonons is much faster in the thin QWI for two reasons:

(i) the acoustic phonon scattering rate is roughly inversely proportional to the cross section of the QWI;
(ii) the inelasticity of electron–acoustic phonon interaction also increases with the decrease of the cross section [6].

One can see from figures 1 and 2 that the electron thermal equilibrium energy for $T = 300$ K is larger than could be expected from $k_B T/2 \approx 13$ meV, while for $T = 77$ K it practically coincides with $k_B T/2 = 3.3$ meV. The difference in thermal equilibrium energies comes from calculation of the electron mean energy in QWIs with a multisubband energetic structure. Approximately one-third of electrons occupy upper subbands in the equilibrium state at a lattice temperature $T = 300$ K due to the Boltzmann distribution. The mean electron energy includes the electron gas kinetic energy ($k_B T/2$) of free motion along the wire and the energy representing the spatial quantization (separation between subbands) in two other directions. In the extreme limit of a thick QWI, when a large number of subbands become occupied, the electron mean energy tends to $(3/2)k_B T$ corresponding to the free-electron gas.

Simulation of hot-electron relaxation dynamics in QWIs demonstrates that intersubband electron scattering primarily by optical phonons leads to a significant carrier redistribution between subbands, and under certain

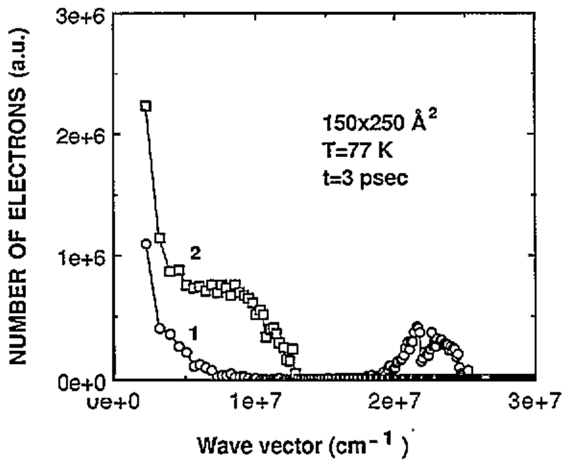

Figure 3. Electron distribution in momentum space in a QWI with a cross section of 150 × 250 Å^2, 3 ps after excitation with $\varepsilon_{ex} = 67$ meV. Curve 1 represents the electron distribution in the first (lowest) subband, curve 2 the distribution in the second subband. The lattice temperature is $T = 77$ K.

excitation conditions intersubband population inversion may occur (compare with the results of [2]). We observe intersubband population inversion when two conditions are fulfilled:

(i) the separation between the two lowest subbands in the QWI is less than the minimum optical phonon (LO or SO) energy, so that electrons cannot be scattered from the bottom of the second subband by the emission of an optical phonon (we demonstrate results for a QWI with a cross section of 150 × 250 Å^2, where this condition is fulfilled);

(ii) electrons are excited just above characteristic energy $\varepsilon = \varepsilon_{02} + \hbar\omega_{LO}$, where ε_{02} is the energy of the bottom of the second subband.

Owing to the significant difference in the number of final states (peak-like density of states near each subband bottom) electrons from both the first and the second subbands are scattered predominantly into the bottom of the second subband after emission of an LO phonon. Figure 3 demonstrates the distribution of electrons in momentum space for the two lowest subbands 3 ps after excitation. Electrons in the first subband are still hot (wavenumbers $k > 2 \times 10^7$ cm^{-1} on curve 1 in figure 3) after emission of an optical phonon and they relax to the bottom of the subband owing to interaction with acoustic phonons. Electrons in the second subband occupy states with smaller wavevectors near the subband bottom, so that strong intersubband population inversion occurs near the centre of the Brillouin zone ($k = 0$) and lasts ≈ 10 ps at a lattice temperature $T = 77$ K. The 'lifetime' of population inversion decreases when T increases because it is defined by the intersubband and intrasubband electron–acoustic phonon scattering rates. Intersubband electron scattering by acoustic phonons is responsible for electron release from the second subband at low temperatures, while intrasubband acoustic phonon scattering leads to the thermalization of the electron distribution.

Summarizing, our simulation reveals a complex dependence of hot-electron gas cooling dynamics on excitation energy in a 1D QWI. Variation of initial electron energy substantially changes the entire picture of hot-electron relaxation owing to electron interaction with various phonons in QWIs. Calculations for electron concentrations less than 10^5 cm^{-1} demonstrate the potential possibilities of two effects: 1D electron gas overcooling and dynamic intersubband population inversion. Electron gas thermalization is much faster in a thin QWI due to increase of the acoustic phonon scattering rate and inelasticity of the electron–acoustic phonon interaction. At low temperatures electrons can be 'trapped' into the upper subbands below the optical phonon energy and stay there for quite a long time defined by intersubband electron–acoustic phonon interaction.

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