Hot-phonon effects on electron runaway from GaAs quantum wires

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Nonequilibrium (hot) optical phonon effects on electron runaway from GaAs quantum wires embedded in AlGaAs have been investigated by Monte Carlo technique. We have simulated the carrier runaway kinetics in the $0<E<1000$ V/cm electric-field range for a lattice temperature of 30 K. Due to optical phonon mode confinement by GaAs/AlGaAs heterointerfaces, the buildup of generated hot phonons is strongly pronounced in the quantum wires. Even at moderate electron concentrations and electric fields, the accumulation of these phonons may become significant and substantially affect all transport properties in the structure. As a result of reduced hot electron cooling rates in the presence of nonequilibrium optical phonons, the high-energy tail of the carrier distribution function extends above the potential barriers at the quantum wire boundaries. This may eventually lead to significant electron escape from the potential well, even at relatively low electric fields, what significantly affects the performance of such nanoscale systems. © *1997 American Institute of Physics.* [S0021-8979(97)02318-9]

I. FORMULATION OF THE PROBLEM

Numerous semiconductor devices benefit from the use of nanostructures. Among those of commercial importance are GaAs/AlGaAs quantum well lasers, specific classes of field-effect transistors, resonant tunneling diodes, avalanche multipliers,[1–6] etc. The performance characteristics of these devices are influenced strongly by hot electron phenomena. Heated electrons in nanostructures generate nonequilibrium optical phonon populations (hot phonons) that cannot escape from the GaAs active regions as a result of confining GaAs/AlGaAs heterointerfaces.[7] Therefore, such nanostructures display much more pronounced hot phonon buildup than bulk semiconductors.[8–16] Nonequilibrium optical phonons strongly affect electron kinetics and transport in nanostructures. For instance, they may impede the performance of the fundamentally new quantum cascade laser,[17] but, being properly employed, could instead improve it.[18,19]

One of the limiting factors of nanoscale quantum well or wire (QWI) device performance is hot electron escape from the potential well.[20] Even at zero electric fields there is always a fraction of electrons on the high-energy tail of the carrier distribution function that are above the potential barriers and can escape into a surrounding quantum wire or well AlGaAs matrix; the higher the lattice temperature and/or electric field, the larger this fraction. But generally, in GaAs/AlGaAs quantum structures at low electric fields the number of such high-energy carriers is negligibly small even at room temperature. There is some critical field, however, at or above which optical phonon emission, the most significant electron relaxation channel in GaAs at moderate electric fields, can no longer be effective in keeping electrons down close to the conduction band bottom. The carriers start to runaway and may eventually escape from a quantum structure.

In this article we demonstrate that nonequilibrium optical phonons can reduce significantly the carrier runaway threshold fields; thus, they have to be taken into account when considering the performance of similar nanoscale devices, incorporating such quantum-well or quantum-wire structure. Our demonstration is based on a 150×250 Å^2 rectangular cross-section GaAs/AlGaAs QWI at $T=30$ K lattice temperature, but the results are qualitatively applicable to any quantum heterostructure with optical phonon confinement within the active region for a wide range of temperatures. QWIs provide striking examples of such phenomena since the influence of hot phonons is especially pronounced in these structures.[9,13,21]

To examine hot optical phonon effects on a quantitative level we have employed the ensemble Monte Carlo procedure[8,21] to perform a self-consistent simulation of a coupled nonequilibrium electron-phonon system.

Our model includes the multisubband electron energy spectrum and the carrier scattering by interface optical, confined longitudinal optical (LO), and acoustic phonons.[22–25] The characteristic strong inelasticity of acoustic phonon scattering in quantum structures[26,27] has been taken into account. It should be pointed out that due to the dominant electron coupling with LO phonons, only these phonons are driven out of equilibrium while interface optical and bulk-like acoustic phonons may be assumed to be in equilibrium.

Electron scatterings by ionized impurities and surface roughness are not included in the present GaAs QWI model. At temperatures around 30 K (and higher) the influence of the latter elastic mechanisms on electron relaxation is insignificant. However, at low temperatures the action of the mentioned processes may contribute considerably to the carrier energy loss rate leading to an increase of the runaway threshold field.

We have considered two different potential wells for electrons of 83.97 and 125.0 meV depth. The latter case corresponds to an Al fraction equal to 0.15 in the GaAs QWI

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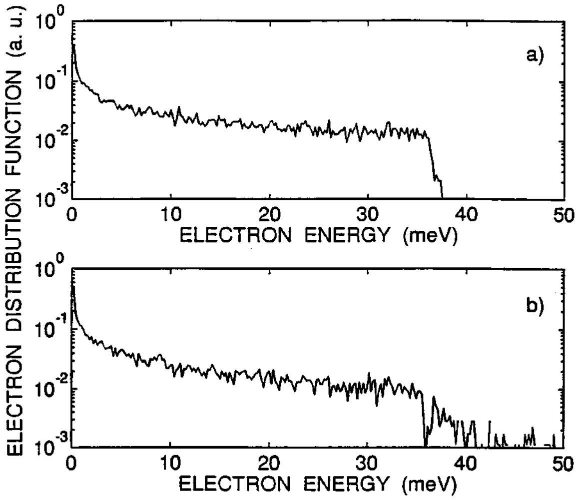

FIG. 1. Electron distribution function vs the mean electron energy at $E=700$ V/cm: (a) the case of negligible optical phonon accumulation in the structure (electron concentration $n_{e1}=1.0\times10^3$ cm^{-1}); (b) the case of well-pronounced hot phonon buildup ($n_{e2}=1.0\times10^5$ cm^{-1}). The GaAs QWI: 150×250 Å^2 rectangular cross-section, $T=30$ K.

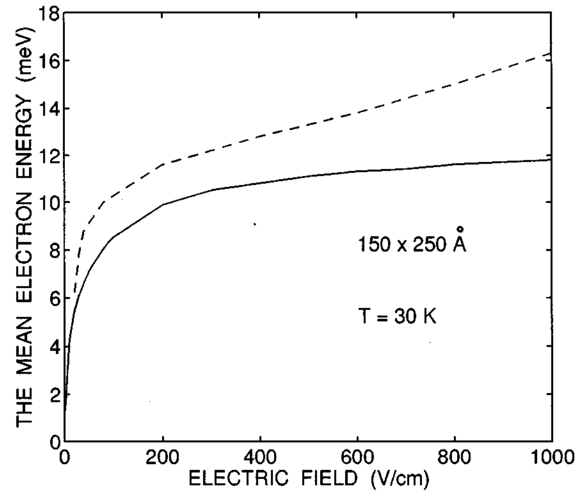

FIG. 2. The mean electron energy dependence on electric field. The solid curve represents the case of negligible optical phonon accumulation in the structure (electron concentration $n_{e1}=1.0\times10^3$ cm^{-1}). The dashed curve corresponds to well-pronounced hot phonon buildup ($n_{e2}=1.0\times10^5$ cm^{-1}). The GaAs QWI: 150×250 Å^2, $T=30$ K.

surrounding AlGaAs material, while in the former case this fraction is 0.1.

II. SIMULATION RESULTS AND DISCUSSION

To demonstrate nonequilibrium optical phonon effects we have performed two sets of the simulations with electron concentrations of $n_e=10^3$ cm^{-1} and 10^5 cm^{-1}. In the former case, hot phonon buildup is negligible and in the latter case it is profound. We will therefore sometimes refer to them as two cases: without and with hot phonons, respectively. Both of these carrier concentrations are describable in terms of nondegenerate electron statistics.

Figure 1 demonstrates the effect of hot LO phonons on the electron distribution function. For low electron concentrations [$n_{e1}=10^3$ cm^{-1}; Fig. 1(a)] the carrier distribution function reflects the streaming regime of electron transport: periodic electron acceleration in the electric field to energies close to the optical phonon energy (≈ 36 meV for GaAs) and subsequent rapid emission of these phonons. As a result, at moderate electric field (below 700 V/cm) electrons do not penetrate significantly beyond the optical phonon energy. In contrast, for high electron concentrations [$n_{e2}=10^5$ cm^{-1}; Fig. 1(b)], there is a considerable population of heated electrons far above the optical phonon energy. This, in fact, is the result of strong buildup of nonequilibrium LO phonon populations and significant reabsorption of these phonons by electrons. Note that the latter situation, in some sense, is similar to the case of high equilibrium lattice temperatures (this similarity is manifest if one neglects the strong anisotropy of the phonon distribution in the momentum space[9]). The hot phonon populations in the case of Fig. 1(b) correspond to approximately 190 K ''effective phonon system temperature'' which is significantly higher than the equilibrium 30 K lattice temperature.

The mean electron energy dependence on electric field is depicted in Fig. 2. Nonequilibrium optical phonons increase significantly the mean electron energy in a wide range of electric fields. The reason is transparent—hot phonons reduce substantially the electron cooling rate. The most efficient electron energy relaxation channel for GaAs, emission of optical phonons, is effectively ''suppressed'' now by the induced LO-phonon reabsorption. Naturally, these effects become even more pronounced at fields above 200 V/cm, where, in contrast, the mean electron energy is close to saturation under equilibrium phonon conditions. This fact indicates that in the case of pronounced nonequilibrium phonon generation in the quantum structure at fields of about 200 V/cm and higher, the scattering mechanisms are not longer effective in preventing electron runaway.

By the same means, hot LO phonons strongly affect electron redistribution among energetic subbands substantially increasing the average energy of the electron subsystem. Figure 3 illustrates these effects on the carrier populations in the two lowest occupied subbands for a 83.97 meV heterobarrier height. In the case of equilibrium phonons (solid curves in Fig. 3) increasing the electric field results in considerable electron heating and transfer to the second energetic subband. However, the carrier population grows there nonmonotonically: for fields above $40-50$ V/cm, when electron motion is pure streaming, optical phonon scattering significantly ''suppresses'' electron transfer to higher energetic subbands. Only at stronger electric fields (above $700-800$ V/cm), optical phonon scattering can no longer prevent electron transfer to the second subband. Pronounced nonequilibrium optical phonon accumulation and reabsorption in the structure destroys the periodic electron motion and also increases substantially the electron system temperature. Therefore, due to a considerable heating at fields above $150-200$ V/cm the electron population in the second energetic subband increases near linearly with growing field as illustrated by the dashed curves in Fig. 3.

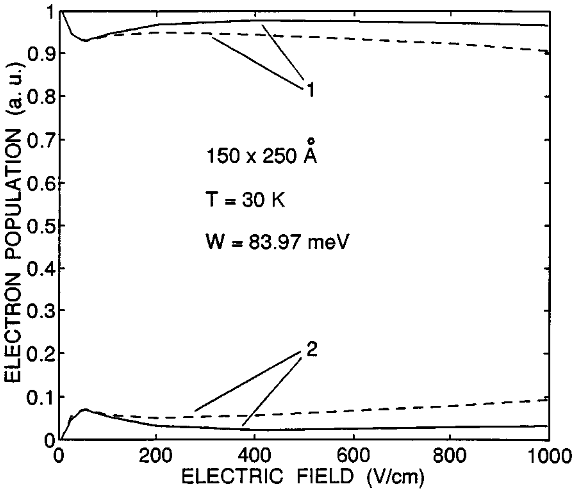

FIG. 3. Electron populations in the first (the lowest) and the second energetic subbands (the upper and the lower curves, respectively) vs electric field. The solid curves correspond to the case of an equilibrium optical phonon system ($n_{e1}=1.0\times10^3$ cm^{-1}), while the dashed curves represent cases with hot phonons ($n_{e2}=1.0\times10^5$ cm^{-1}). The potential heterobarrier height, W, is approximately 83.97 meV.

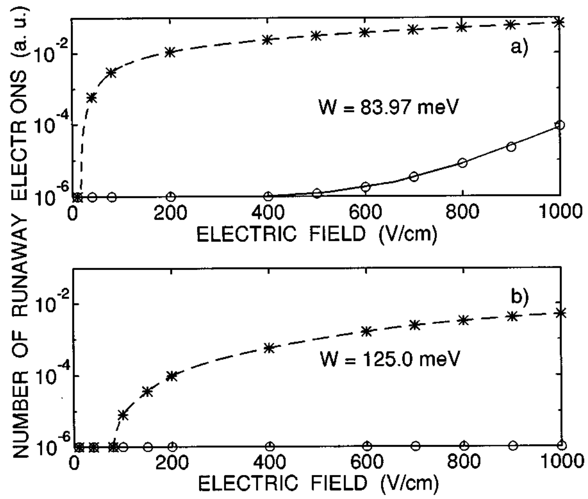

FIG. 4. Number of runaway electrons vs electric field. The solid curves with empty circles represent the case of negligible optical phonon accumulation in the structure (electron concentration $n_{e1}=1.0\times10^3$ cm^{-1}). The dashed curves with stars correspond to well-pronounced hot phonon buildup ($n_{e2}=1.0\times10^5$ cm^{-1}): (a) GaAs/$Al_{0.1}Ga_{0.9}As$ potential barrier height, W, is approximately 83.97 meV; (b) GaAs/$Al_{0.15}Ga_{0.85}As$ potential barrier height is $\approx$125.0 meV. The GaAs QWI: 150×250 Å^2, and $T=30$ K.

It is evident that the nonlinear phenomena considered are so profound that they must play a crucial role in semiconductor devices based on electron intersubband transitions. Consequently, the performance of all quantum well lasers and particularly quantum cascade lasers[17–19] is influenced strongly by nonequilibrium optical phonon populations.

To investigate hot optical phonon effects on the electron escape from the GaAs/AlGaAs quantum wire we have calculated the number of electrons above the potential barriers in the cases with and without nonequilibrium phonons. Obviously, not all the electrons that runaway above these barriers will eventually escape from the active region. It is necessary for those carriers to undergo additional scattering and real space transfer processes in order to transit from confined quasi-one-dimensional states within the GaAs quantum wire to quasi-two- or quasi-three-dimensional states in the AlGaAs barrier material. Some electrons will be scattered to lower energies by optical phonon emission or by any other efficient scattering at the wire interface preventing such a transition. As a result, part of escaping electrons will be eventually captured back into the quantum wire. However, due to greatly increased electron scattering rates and a significant energy portion gained in the presence of nonequilibrium optical phonons the carrier escape processes are enhanced dramatically and dominate in the system.

The simulation results are plotted in Figs. 4(a) and 4(b) for two different heterobarrier heights corresponding to different compositions of the barrier material (AlGaAs). For the case with hot phonons, at an electric field of 200 V/cm a significant fraction of electrons is already above the 83.97 meV barrier [Fig. 4(a)], whereas any detectable carrier runaway occurs only at fields above 400 V/cm in the case of equilibrium phonons. For the higher potential barrier height of 125.0 meV at the GaAs wire boundaries, the effect is, naturally, even more profound [Fig. 4(b)]. Note that in both considered cases, only a negligible fraction of electrons can escape from the quantum wire at fields up to 1000 V/cm if nonequilibrium optical phonon generation is insignificant in the structure. Consequently, hot optical phonons do not impede the performance of quantum wire devices with operational electron concentrations less than 10^3 cm^{-1}. If, however, this concentration is close to or exceeds 10^5 cm^{-1}, nonequilibrium optical phonons greatly reduce the upper electric field limit of such nanoscale device operation; indeed, this field limit is reduced to $100-200$ V/cm for the case of the 83.97 meV heterobarrier height.

III. SUMMARY

In summary, we have performed numerical simulations of electron runaway from a 150×250 Å^2 GaAs/AlGaAs quantum wire at $T=30$ K lattice temperature.

For electron concentrations in the active region of about 10^5 cm^{-1}, the strong buildup of nonequilibrium optical phonons results in a dramatic decrease of the critical electric field at and above which the electron runaway occurs. This runaway leads to the carrier escape from the quantum wire that may significantly impede the performance of nanoscale devices fabricated with similar quantum-wire structures.

The estimated effective ''phonon temperature'' in the presence of nonequilibrium phonon populations is as high as approximately 190 K at 700 V/cm field. This means that at temperatures around 30 K and even higher, hot phonon effects are very strong even at moderate electric field.

The simulations have been performed for a specific quantum wire; however, the results obtained have a more general meaning. Hot phonon buildup is well pronounced in any heterostructure-based quantum structure with confined electron and optical phonon systems.[7,22] Therefore, it should be accurately taken into account when designing or modeling a number of active elements such as nanoscale hot electron devices and devices operating on the basis of intersubband carrier transitions.

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