Monte Carlo study of GaN versus GaAs terahertz quantum cascade structures

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Due to their large optical phonon energies, nitride semiconductors are promising for the development of terahertz quantum cascade lasers with dramatically improved high-temperature performance relative to existing GaAs devices. Here, we present a rigorous Monte Carlo study of carrier dynamics in two structures based on the same design scheme for emission at 2 THz, consisting of GaN/AlGaN or GaAs/AlGaAs quantum wells. The population inversion and hence the gain coefficient of the nitride device are found to exhibit a much weaker (by a factor of over 3) temperature dependence and to remain large enough for laser action even without cryogenic cooling. © 2008 American Institute of Physics. [DOI: 10.1063/1.2894508]

Technological development in the terahertz spectral region has so far been limited, as conventional device concepts from both the electrical and the optical domain cannot be readily extended to operation at terahertz frequencies. Yet, the potential of terahertz radiation in numerous fields, including medical diagnostics, security screening, and manufacturing quality control, has recently been identified and is driving extensive research efforts to develop the required components. In the area of terahertz sources, a promising approach is provided by the quantum cascade (QC) laser scheme based on intersubband (ISB) transitions in semiconductor quantum wells (QWs). In this lasing modality, the emission wavelength is tailored through the design of the multiple-QW active material and thus can be tuned by design over a broad spectral range. Terahertz QC lasers based on GaAs/AlGaAs QWs have, in fact, been developed in the past few years and currently span the 1.2–5 THz range with peak output powers often on the order of a few tens milliwatts.1–5

Although these advancements are impressive, the operation of GaAs/AlGaAs terahertz QC lasers fundamentally requires cryogenic cooling, with maximum temperatures reported so far near 170 and 120 K for pulsed and continuous-wave emission, respectively.2 This important limitation is related to an intrinsic property of the GaAs/AlGaAs material system, namely, the presence of longitudinal optical (LO) phonons with energies $h\nu_{LO}$ relatively close to the room-temperature thermal energy $k_BT$ of 26 meV (e.g., $h\nu_{LO} \approx 36$ meV in GaAs). As a result, laser action at or near room temperature is precluded by the process of thermally activated LO-phonon emission. This nonradiative decay mechanism is illustrated schematically in Fig. 1, where the traces labeled $|\mu\rangle$ and $|\ell\rangle$ denote the upper and lower laser subbands, respectively. At cryogenic temperatures, a large population inversion can be established since the majority of electrons in $|\mu\rangle$ occupy states near the bottom of the subband, from which they cannot decay nonradiatively into $|\ell\rangle$ via LO-phonon emission because of the requirement of energy conservation. As the temperature is increased, however, more and more electrons in $|\mu\rangle$ can gain enough thermal energy that scattering into $|\ell\rangle$ via LO-phonon emission becomes allowed. Since these scattering processes are ultrafast, the end result is a dramatic reduction in the device population inversion and optical gain. A recent experimental study has concluded that this mechanism is indeed the main factor limiting the maximum operating temperature of GaAs/AlGaAs terahertz QC lasers.5

This argument suggests the exploration of novel semiconductor heterostructures having larger LO-phonon frequencies as a means to improve the high-temperature performance of terahertz injection lasers. One promising system currently attracting considerable attention for various applications of ISB transitions is that of GaN/AlGaN QWs, where the LO-phonon energies lie in the 91–99 meV range. As a result, in a GaN-based terahertz QC laser, the breakdown in device performance due to the onset of thermally activated LO-phonon emission can be expected to occur at much higher temperatures. Previous theoretical studies, based on rate-equation models of varying complexity, have suggested that even room-temperature terahertz lasing may be feasible with III-nitride QWs.6,7 The goal of this work is to provide a rigorous comparison between GaAs/AlGaAs and GaN/AlGaN terahertz QC structures where both material systems are treated on equal footing, in order to properly quantify the potential for improvement offered by the latter system.

To that purpose, we employ a microscopic model of carrier dynamics in QC gain media based on a set of Boltzmann-like equations solved with a Monte Carlo technique.8–11 Unlike rate-equation models (even those including carrier-carrier scattering), this approach allows us to fully take into account the presence of nonequilibrium carrier distributions in QC gain media and their effect on the ISB scattering rates. This is particularly important in the description of terahertz QC lasers, where electron-electron scattering (which strongly depends on the global carrier distribution) plays a prominent role in determining the population inversion. Additionally, in order to obtain the fairest possible comparison between the two material systems under consideration, we have carried out simulations of two QC structures based on the same design scheme5 and with the same target emission frequency of 2 THz (8.2 meV), one consist-
The two QC gain media were designed using a Schrödinger-equation solver based on the effective-mass approximation, with the characteristic built-in electric fields of nitride heterostructures included explicitly. Shown in Figs. 2(a) and 2(b) are the conduction-band profiles and squared envelope functions of the relevant bound states of the GaN and GaAs structures, respectively, under optimal bias conditions. The optical transitions occur between the states labeled [1] and [2] in each period of these active materials. The lower laser states are rapidly depopulated through tunneling into state [2] downstream and scattering into state [1] via resonant LO-phonon emission. To maximize the speed of the latter process, in both structures, the energy separation between subbands [1] and [2] is close to the LO-phonon energy of the well material. This QC design scheme has been successfully demonstrated in a recent GaAs/AlGaAs device and was chosen for this study because of its inherent simplicity as it contains only three QWs per repeat unit. In the GaN structure, the intrinsic piezoelectric fields were computed assuming an Al0.07Ga0.93N strain-balancing growth template. It should be noted that GaN wells and Al0.15Ga0.85N barriers grown on such template are under relatively low strain.

In our simulations, a particle-based Monte Carlo approach is used to determine the steady-state carrier distributions of the laser subbands as a function of temperature, starting from a constant population initially assigned to each subband. The numerical model includes four subbands per period, and a total of three adjacent periods is simulated. Periodic boundary conditions are applied such that for each particle exiting the third repeat unit, a new one is injected in the first. Electron/electron and electron/LO-phonon scattering are both included in the simulations, with the relevant scattering rates at a given temperature computed and stored for each subband pair for a discrete number of initial electron energies. During the Monte Carlo simulation, an interpolation is used to determine the rates at arbitrary initial energy values. The electron final state after scattering with a LO phonon is determined using a rejection technique on the scattering angle probability distribution, which is precomputed as a function of the electron initial energy, stored, and used as a two-dimensional look-up table. The final state after an electron/electron scattering event is obtained using a multiple-rejection approach, and the relevant probability distribution is generated using the four-subband overlap integrals. Particularly critical is the treatment of screening, and in this work we employ a temperature-dependent single-subband screening approach.

In Fig. 3, we plot the calculated fractional population inversion \( \Delta n = (n_e - n_h)/n_{00} \) versus temperature for the two...
structures of Figs. 2(a) and 2(b). Here, \( n_d \) and \( n_3 \) are the sheet electron densities of the upper and lower laser subbands, respectively, and \( n_{\text{tot}} \) is the total electron density per period, taken to be \( 2 \times 10^{10} \text{ cm}^{-2} \). The results shown in this figure fully support and quantify the claim that GaN terahertz QC gain media can provide better performance compared to GaAs devices. In particular, \( \Delta \omega \) in the GaN structure is found to degrade much more slowly with increasing temperature compared to the GaAs device. For example, as the temperature is increased from 10 to 300 K, \( \Delta \omega \) in the GaN structure decreases only by a factor of 1.25 versus 4.48 in the GaAs gain medium. These numerical results are consistent with the severe performance degradation with increasing temperature experimentally observed in GaAs terahertz QC lasers, which is caused by thermally activated LO-phonon emission and (to a lesser extent) by thermal backfilling of the lower laser states [3] from the states [1] downstream. Both of these limiting factors are much less effective in the presence of the large LO-phonon energies of nitride QWs, as clearly indicated by our simulation results.

The maximum operating temperature of the two gain media can be estimated from the plots of Fig. 3 as the temperature beyond which \( \Delta \omega \) is increased from 10 to 300 K, \( \Delta \omega \) in the GaN structure is found to degrade much more slowly with increasing temperature compared to the GaAs device. For example, as the temperature is increased from 10 to 300 K, \( \Delta \omega \) in the GaN structure decreases only by a factor of 1.25 versus 4.48 in the GaAs gain medium. These numerical results are consistent with the severe performance degradation with increasing temperature experimentally observed in GaAs terahertz QC lasers, which is caused by thermally activated LO-phonon emission and (to a lesser extent) by thermal backfilling of the lower laser states [3] from the states [1] downstream. Both of these limiting factors are much less effective in the presence of the large LO-phonon energies of nitride QWs, as clearly indicated by our simulation results.

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