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Hot electrons in quantum cascade lasers

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Abstract. We have developed a theory describing the operation of lasers based on intersubband transitions in a quantum well. The theory combines a first-principles description of the intersubband lineshape and the optical gain with kinetic models for carrier heating. The theory is consistent with the experimental data available and suggests new ways of improving the laser design for room temperature operation with high output power. At low carrier concentrations, it is possible to achieve positive values of the gain at room temperature even in the absence of an overall population inversion between quantum well subbands. For higher (but still moderate) concentrations, the theory predicts a peculiar dependence of the output wavelength on the pump current, including a regime where the lasing wavelength switches "digitally" between two stable values.

The quantum cascade laser is a new mid-infrared laser, based on unipolar transitions of electrons between energy levels created by quantum confinement. Since the first demonstration of QCL (Faist et al. 1994), its design has continuously improved through a series of elegant innovations by the Bell Labs group (Faist et al. 1995a,b) culminating in their recent report of a high power room-temperature operation (Faist et al. 1996).

The device has multiple periods (25 in reported structures) and each electron performs a cascade of transitions down the periodic ladder. Under the operating conditions, each period must have net zero charge: by Gauss' law this is necessary in order that subsequent periods could replicate each others electrostatic state. To avoid the space charge accumulation, associated with current flow, one therefore needs a reservoir of positive fixed charge, compensating the negative mobile charge in each period. Introduction of such a reservoir, implemented as a doped superlattice region is the key design innovation that led to the successful implementation of a unipolar laser. Subsequent QCL designs entrusted the reservoir with an additional mission to suppress the unwelcome tunneling from the upper level into the continuum. For this purpose, the superlattice is implemented as an electronic Bragg filter with a stop band in the range of energies of upper level states (Faist et al. 1995). Thus, most carriers enter the QW only via the upper and leave only via the lower subband, while leakage from the upper subband directly into the reservoir is negligible.

We have carried out a theoretical analysis of the QCL operation (Gelmont et al., 1996; Gorfinkel et al., 1996). This analysis will not be reproduced here; instead we confine ourselves to a brief discussion.

Our analysis suggests that QCL operation is dominated by hot-electron effects. Non-equilibrium electron distributions arise from the power $\mathcal{P} \approx J \cdot \hbar\Omega$ per unit area, dissipated in each cascade period. The energy is stored in the *transverse degrees of freedom*, corresponding to in-plane motion of carriers and it fundamentally changes the lineshape of intersubband resonance and the spectral characteristics of gain. Transverse relaxation of the intersubband resonance and the hot-carrier effects are indispensable for the correct physical understanding of the temperature behavior of quantum cascade lasers.

Conventional two-level model does not adequately describe the intersubband gain function in experimentally realized QCL heterosystems. The reason is two-fold. Firstly, one cannot neglect the nonparabolicity: its inclusion suppresses the peak gain value by more than an order of magnitude. Secondly, the relaxation rate of intersubband resonance, which is mainly due to transverse intrasubband scattering processes, is strongly dependent on electron kinetic energy, $\gamma = \gamma(E)$. Indeed, the rate of optical phonon scattering has a threshold nature: when $E > \hbar\omega_{op}$ it increases by nearly an order of magnitude due to the onset of intrasubband emission.

The generalized expression for the intersubband gain at an optical frequency Ω is of the form (Gelmont et al. 1996):

$$g(\Omega) = \frac{4e^2 |z_{12}|^2 m_2 \Omega}{\hbar^3 a\, c\sqrt{\kappa_\infty}} \int_0^\infty \frac{d\varepsilon\, \gamma(\varepsilon)\,[f_2(\varepsilon) - f_1(\varepsilon_1)]}{[\Omega - \Omega_\varepsilon]^2 + [\gamma(\varepsilon)]^2} \quad , \tag{1}$$

where Ω_ε is the optical transition frequency for the in-plane electron momentum $\hbar k = \sqrt{2m_2\varepsilon}$, viz. $\hbar\Omega_\varepsilon \equiv \hbar\Omega_0 + \varepsilon_2 - \varepsilon_1$, where $\varepsilon_2 \equiv \varepsilon$ and $\varepsilon_1 = \hbar^2k^2/2m_1$ are kinetic energies in the upper and lower subbands, respectively, characterized by the effective masses m_2 and m_1 and the distribution functions f_2 and f_1. The function $\gamma(\varepsilon)$ describes the transverse phase relaxation rate due to intrasubband scattering, both elastic and inelastic.

Depending on the laser design, there may be different scenarios of how this energy is distributed among various electrons and dissipated into the lattice. It is worthwhile to stress that Eq. (1) does not rely on the electron temperature approximation and remains valid for general electron energy distributions within each subband. Validity of Eq. (1) is not restricted to any particular scattering mechanism responsible for the transverse phase relaxation.

The most attractive situation arises at low carrier concentrations ($n_D \ll 10^{11}$ cm^{-2}) when electron-electron collisions are not fast enough to establish a common electron temperature T_e between the two subbands. It turns out that in this regime the lower-subband electron distribution can be approximately characterized by a negative temperature,[1] so that states near the subband bottom are mostly unoccupied. At the same

1. For high positive temperatures the electron distribution becomes uniform over the entire subband. For $T_e < 0$ the distribution is inverted, the lower energy states having smaller occupation probability; one can say that negative temperatures are higher than $T_e = \infty$,

time, the upper subband remains approximately in a thermal ensemble, characterized by the ambient temperature. This situation is most favorable for high gain. It is even possible to achieve high positive values of $g(\Omega)$ at room temperature without an overall population inversion between the two subbands. Within the framework of our theory, the low concentration regime can be treated rigorously.

For higher (but still moderate, $n_D \lesssim 10^{11}\,\mathrm{cm}^{-2}$) concentrations, the T_e approximation becomes applicable, but it is still possible (at least semi-quantitatively) to regard optical phonon scattering as the dominant phase breaking mechanism. In this range, we predict a peculiar hot electron effect, manifested in the dependence of the lasing wavelength λ on the pump current, including a regime where λ switches "digitally" between two stable values.

Very high concentrations ($n_D \gg 10^{11}\,\mathrm{cm}^{-2}$) require a special consideration, as it becomes necessary to explicitly include electron-electron scattering in the calculation of $\gamma(\varepsilon)$. Also the energy balance equation in this range should include the dependence of the electron cooling rate on the carrier density and effective temperature due to optical phonon bottleneck. Moreover, as shown by Warburton et al. (1996), at high carrier concentrations the nonparabolicity is strongly suppressed by depolarization, so that intersubband resonance becomes a collective effect. Our theory does not directly apply to the high-concentration limit.

Experimentally reported QCL heterostructures (Faist et al. 1994-1996) operate neither in the high-concentration nor in the low-concentration regime. For moderate concentrations our theory provides a semiquantitative account of all experimentally observed features, such as the existence of a sharply defined critical temperature beyond which the QCL does not reach the generation regime. This is due to the fact that the subthreshold gain is not a monotonic function of the injection current in QCL but reaches a maximum and then declines due to the hot-carrier effect. Above threshold, the dependence of gain on T_e leads to a lower than expected slope efficiency of the laser.

At moderate concentration it is also possible to have a positive gain even in the absence of inversion between the two subbands, i.e. for $n_1 \gtrsim n_2$. This effect, recently observed by Faist et al., occurs owing to the non-parabolicity ($m_2 > m_1$). At a sufficiently high wavevector k, the occupation probability of state $\varepsilon_2(k)$ in the upper subband is higher than that of state $\varepsilon_1(k)$, even though the lower subband has higher overall population. This can be also seen in a different way: in the regime, where both subbands are characterized by the same effective temperature, it is possible to introduce the subband quasi-Fermi levels E_{F_1} and E_{F_2} for the distributions f_1 and f_2, respectively. One can then show that the range of $g(\Omega) > 0$ corresponds to the relation $\hbar\Omega < E_{F_2} - E_{F_1}$, familiar from the theory of conventional semiconductor lasers (Bernard and Duraffourg, 1961).

In contrast, the existence of a positive gain for $n_1 > n_2$ at low concentrations does not depend on the nonparabolicity and is a much stronger effect predicted in our theory. The low concentration regime offers possibility of higher performance, because the carrier heating effects in this case actually improve the effective population inversion for states participating in the lasing transition.

Given the tremendous applications potential of the QCL, we believe the device deserves a major development effort. The improvement strategies that have born most fruit so far, have dealt with the kinetics of subband population and with the laser engineering, such as improved heat sink, cavity design, etc. We have identified three new strategies. First, one should strive to reduce the effects of non-parabolicity by employing new material systems and designs to engineer subbands with approximately equal kinetic masses in the QW plane. Next, one can attempt to reduce the carrier heating effects by introducing new carrier cooling channels, e.g., via intervalley phonon emission in the doped reservoir region. Third, one can render hot-carrier effects harmless by implementing the low concentration regime of operation. Our work shows that the QCL still has an enormous reserve for improvement.

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