The Effects of Temperature on the Gain Profile of THz Quantum Cascade Lasers

Rikard Nelander† and Andreas Wacker
Division of Mathematical Physics, Physics Department
Lund University
Box 118, 22100 Lund, Sweden
† Email: rikard.nelander@fysik.lu.se

***Abstract*— We study the rapid decrease of peak gain in THz Quantum Cascade Lasers (QCLs) with increasing temperature. The effect of various microscopic scattering processes on the gain profile as a function of temperature is discussed. We argue that increased broadening, primarily due to increased impurity scattering, and not diminishing population inversion, is the main reason for the reduction of peak gain.**

I. Introduction

Extending the operating region of THz QCLs towards room-temperature crucially depends on a quantitative understanding of the various temperature effects. In order to study these effects the THz QCL in Ref. [1] has been simulated. It is a four-well design, see Fig. 1, emitting at 1.9 THz (7.9 meV) at a bias of 46.5 meV/period and lased up to 95 K in continuous mode.

II. Theory

Our calculations are based on Non-Equilibrium Greens Functions (NEGF) which satisfy the Dyson Equation and the Keldysh Relation [2], [3]. This method can be seen as an extension of density matrix theory to take into account broadening and scattering in a systematic manner. Our approach is free of fitting-parameters and depends only on well-known material data. We include electron-phonon, impurity and interface roughness scattering within the self-consistent first order Born approximation, and electron-electron interaction within the mean field approximation. The gain is calculated according to Ref. [4]. In our model the temperature enters in two ways; (*i*) The occupation of phonon modes, and (*ii*) in the Debye approximation for the screening of ionised impurities.

III. Results

For the operating bias of 46.5 mV/period we obtain a current of 170 A/cm^2 at low temperatures which agrees well with the experimental current of 150 A/cm^2. The corresponding gain spectra are shown in Fig. 2. The gain peak at 9 meV is strongly reduced with increasing temperature, in agreement with the observed vanishing of lasing at 95 K. A similar behaviour is found for the absorption peak at 14 meV, which corresponds to absorption between state 4 and 5.

Commonly the disappearing gain is related to the vanishing of population inversion. Fig. 3 shows that the population difference between the relevant levels, 3 and 4, indeed decreases with temperature. We also plotted the occupation in state 3 assuming thermal equilibrium and that 90 % of the carriers occupy state 1. The similar shape of the two curves suggests that thermal backfilling essentially stands for the reduction in population inversion. The fact that the lower laser state is

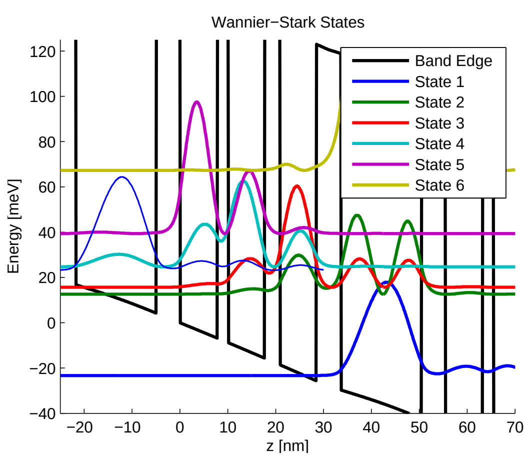

Fig. 1. Conduction band profile with the six lowest Wannier-Stark states per period. For clarity the lowest state for the previous period is plotted. The lasing transition occurs between state 3 and 4.

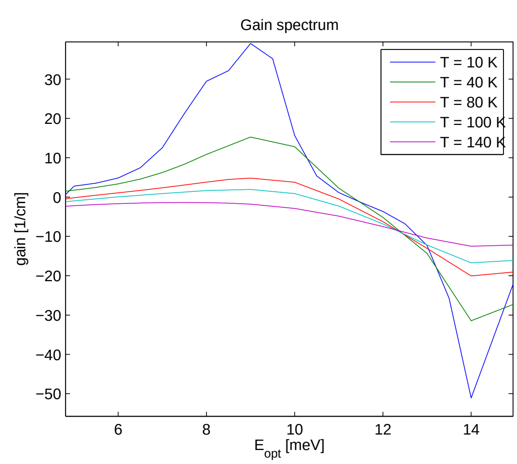

Fig. 2. Total gain for different temperatures

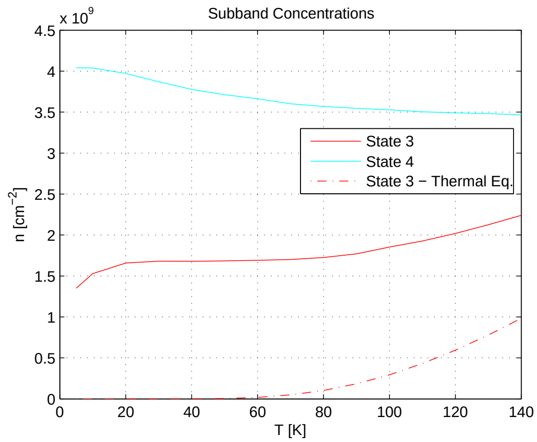

Fig. 3. Subband concentration as a function of temperature for the two lasing state. The population of the lower laser state assuming thermal equilibrium with state 1 is also plotted.

separated from the heavily populated state 1 by approximately the optical phonon energy suggests that this effect becomes relevant only at temperatures far above 100 K. Therefore this decrease in population inversion is much less compared to the significant reduction of gain in the studied temperature range.

The excess reduction in peak gain can be related to a change in line shape. Indeed, Fig. 2 shows that the gain transition is broadened with temperature, which reduces its peak value. The same holds for the absorption transition which overlaps with the gain region at higher temperatures causing an additional reduction of gain.

IV. Discussion of broadening mechanisms

The width of the gain peak is related to scattering induced broadening. The mechanisms included are:

Optical phonon emission, the dominant scattering effect in most QCLs, is proportional to $n_B(\hbar\omega)+1$ where $n_B(\hbar\omega)$ is the Boltzmann-factor at the optical phonon energy. The phonon absorption rate is proportional to n_B. At $T = 100$ K we have $n_B \sim 10^{-2}$ for an optical phonon energy of 36.7 meV. Thus spontaneous optical phonon emission is by far the most dominant process which does not depend on temperature.

Acoustic phonon scattering contributes very little to the total scattering. Assuming elastic scattering and high temperature compared to the typical acoustic phonon energy one can show that the acoustic phonon scattering contributes less than 1 % to the total elastic scattering and can therefore be neglected.

Impurity scattering is strongly influenced by the screening of ionized dopants by electrons, which is a complex many-body problem. Treating it correctly is a formidable numerical task [5]. A common simple approach is the Debye-approximation where the electrons contributing to screening is assumed to be in thermal equilibrium and obey Boltzmann statistics. This results in a temperature dependent screening length

$$\lambda^2_{\mathrm{Debye}} = \frac{e^2 n_{\mathrm{3D}}}{\epsilon_s \epsilon_0 k_B T} \tag{1}$$

where n_{3D} is the average electron concentration, $\epsilon_s\epsilon_0$ the dielectric constant of the sample. The idea is that a hot electron gas is less affected by the impurity potential and will therefore screen it less. For simplicity, the temperature of the electron gas has been approximated by the substrate temperature, in this study.

V. Conclusion

We have shown that although lasing stops at around 100 K, a large proportion of the population inversion remains. The further reduction of gain can be related to increased broadening. Our analysis indicates that the temperature dependence of impurity scattering due to screening is the dominant effect.

References

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