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# Modelling of three-well extraction-controlled terahertz frequency quantum cascade lasers using an extended density matrix approach

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## 1. Introduction

Since their first demonstration more than a decade ago, terahertz frequency quantum cascade lasers (THz QCLs) [1] have become important compact sources of coherent radiation in the 1.2–5.2 THz band, with peak pulsed output power of 1 W [2] and a maximum operating temperature of ~ 200 K [3]. High temperature THz QCLs are usually based on the resonant tunnelling injection scheme, in which the injected carriers are extracted rapidly by thermally activated longitudinal optic (LO) phonon scattering, leading to the device performance degrading at elevated temperatures. To improve the temperature performance, an alternative scheme has been proposed in which LO-phonon scattering is used to obtain a strong carrier injection [4-6], and a simple 'extraction-controlled' THz QCL design [7] based on this scheme has been demonstrated experimentally [8]. However, these designs have not yet yielded high operating temperature (>170 K), and carrier transport modelling is desirable for further improvements. Here, an extended density matrix (DM) model [9] is employed to develop an understanding of carrier transport in a three-well extraction-controlled THz QCL, and the mechanisms limiting their temperature performance are discussed.

## 2. Numerical results

The extended DM approach is capable of modelling QCLs with an arbitrary number of subband levels, and there is no need to select an injector subband manually in advance. This is in contrast with other DM models and is beneficial to the investigation of the bias evolution of carrier transport. The subband wavefunctions for one period were calculated based on the tight-binding model, and these localized wavefunctions were shifted to upstream and downstream neighbouring periods in our DM approach. We assume that carrier transport is only determined by interperiod resonant tunnelling and intraperiod scattering. As shown in Fig. 1 (a), only three bound subbands are considered within each period, and are assigned the labels 3, 2, and 1, corresponding to the injector level, upper laser level and lower laser level, respectively.

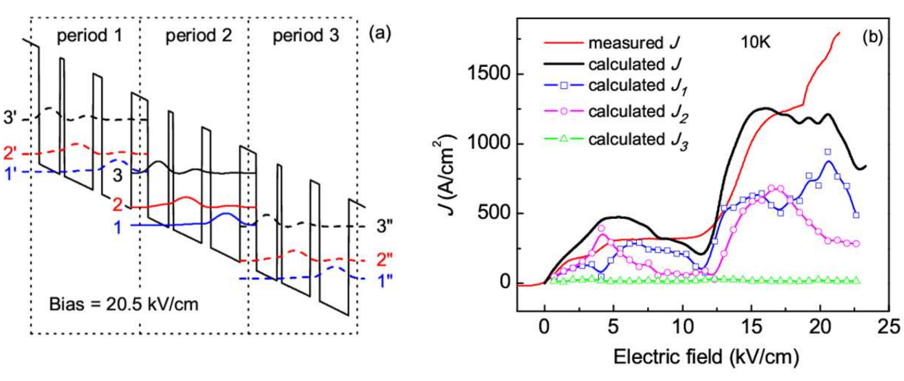


Fig. 1. (a) Calculated conduction band diagram and squared moduli of bound electronic wave functions of a three-well design at an electric field of 20.5 kV/cm. (b) Comparison between the calculated and measured I–V curves, and the calculated resonant tunnelling current from each subband to the downstream period versus electric field. $J_1$ $J_2$ and $J_3$ indicate the current density extracted from the subband levels 1, 2 and 3, respectively.

The calculated and measured I–V curves are compared in Fig. 1 (b). Effects of photon driven carrier transport were included in the calculation of the I–V curve. A voltage drop of 2.5 V due to the Schottky barrier was subtracted and a series contact resistance of 0.3 Ω was added to calibrate the measured I–V curve. The calculation shows a good agreement with the experimentally measured values, especially for the two current peaks at the electric field of 4.8

and 15.7 kV/cm. Our DM approach allows the analysis of parasitic current paths. The current extracted to the downstream period originates mostly from levels 1 and 2, while the current from level 3 is much smaller. This indicates a parasitic path for the carrier transport, i.e., from the upper laser level 2 to the next period. The current from this parasitic path peaks at an electric field of 17 kV/cm, corresponding to the alignment between the upper laser level and the extractor level (also the injector level of the next period). This effect raises the current density and lowers the gain of the design significantly.

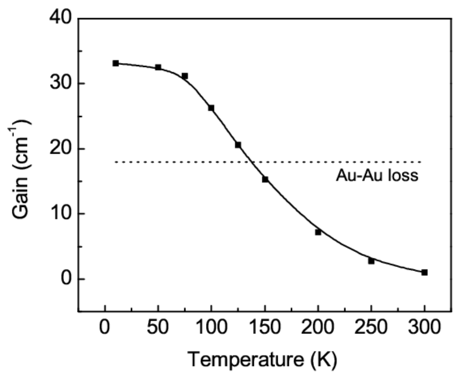


Fig. 2. Calculated unclamped peak gain of the design as a function of the lattice temperature. The dotted line shows the calculated optical loss in a QCL with a gold–gold waveguide configuration.

With increasing temperature, the degradation of performance can be attributed to the decrease in extraction strength, the loss of upper laser level population, and the reduction in injection efficiency. As shown in Fig. 2, the calculated maximum operating temperature is 137 K, a little higher than the measured 123 K. This indicates that temperature degradation is underestimated slightly, which may be due to continuum subbands and interperiod scattering being neglected in our model.

## 3. Conclusions

An extended density matrix approach has been applied to a three-well extraction-controlled THz QCL. Carrier transport and the temperature effects were investigated. A parasitic path from the upper laser level has been identified as the principle reason for the large current and the limited operating temperature, and this improved understanding will underpin future improvements in scattering-injection QCL designs. Details of this parasitic carrier transport and the methods to avoid it will be discussed.

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