Optimization of MBE Growth Parameters for GaAs-based THz Quantum Cascade Lasers

A.M. Andrews\(^1,2\), T. Roch\(^2\), A. Benz\(^1\), G. Fasching\(^1\), W. Schrenk\(^2\), K. Unterrainer\(^1\), G. Strasser\(^2\)

\(^1\) Institut für Photonik, 
\(^2\) Institut für Festkörperphysik und Zentrum für Mikro- und Nanostrukturen, Technical University of Vienna, A-1040 Wien

Introduction

Solid state terahertz (THz) lasers were made possible through the rapid progress in quantum cascade lasers (QCLs) \[1\]. Despite the advances in mid-infrared (MIR) QCLs \[2\], THz QCLs remain difficult to fabricate. The tolerances in alloy composition, layer thickness, and doping are lower for THz QCLs than their MIR counterparts. Typical THz structures can require more than a day to grow by MBE and a thickness change of a few percent will result in a non-lasing device.

In our QCL active region design, we use the phonon depletion scheme, shown in Fig. 1, to quickly depopulate the lower lasing level \[3\], to produce THz lasers that work above the critical liquid nitrogen temperature.

![Figure 1: Schematic of the conduction band structure (GaAs and Al\(_{0.15}\)Ga\(_{0.85}\)As) and electron wave functions in one unit cell of a 15 µm THz QCL active region with 271 cascade periods. This dual-wavelength design, 98.2 and 118.9 µm, results from the laser transitions from level 4 to 2 and 3 to 2. The rapid transition from level 1 to 5' emits one LO phonon.](image-url)
Experiment and Results

The GaAs-based THz structures [4] were grown by solid-source molecular-beam epitaxy (MBE) in a modular GEN II. The MBE system has a vertical wagon wheel source configuration with four upward and four downward facing cells. Samples were grown on semi-insulating 3-inch GaAs substrates. Typical growth conditions used were substrate temperatures between 590 – 610°C with an As4 pressure of 8x10^-6 Torr. Original configuration, A, for the system was AC power supplies for all sources with the dual-filament Ga cell in the most upward facing position and the conical Al cell in the least upward facing position, approximately 90° from the Ga cell. The final configuration, B; uses a DC power supply for the Ga and exchanges the conical Al cell with a SUMO Al cell.

Due to the relatively low thickness tolerances, careful attention to growth conditions and their effect on wafer uniformity must be measured. Growth rate calibrations were first determined by reflected high energy electron diffraction (RHEED) oscillations and then further refined by the growth of either a single superlattice or double superlattice measure ex-situ by high resolution x-ray diffraction (XRD). Shutter operations change the heat load of individual sources required to maintain specific cell temperatures by reflecting heat back into the cell. For example, the Ga cell initial growth rate upon opening the shutter was determined to be -10% of the steady state growth rate with a characteristic decay time of around 15 seconds. A second source of thickness error comes into account when growing 10 – 15 µm structures, and that is source material depletion. Due to the relatively low Al content of 15%, only the Ga depletion needs to be determined. By growing a growth rate calibration before and after the THz structure, the Ga depletion was measured to be 1% for every 10 µm of growth.

Due to the orientation of the sources, a non-rotated sample results in a thickness gradient of the desired thickness of +19% at the leading edge of the substrate to -21% at the trailing edge of the substrate for each source. This was confirmed by XRD for the growth of a non-rotated superlattice. Rotating the sample creates a more even thickness distribution across the wafer with a minimum every half rotation. After four rotations per epilayer, the average thickness error is slightly less than -1% at the edge. The total growth rate should be adjusted accordingly to maximize the usable area of the wafer when using epilayers on the order of a few or fractional monolayers.

N-type doping calibrations in the 10^{15} – 10^{16} cm^-3 range are critical for THz QCLs, so a 4 µm Si-doped GaAs layer is grown on a semi-insulating Al_{x}Ga_{1-x}As barrier and GaAs substrate for each calibration. After 3 – 5 samples are measured, this produces reliable doping profiles with a 10% error.

Initial THz structures were grown with system configuration A, which produced broad peaks in XRD due to poor Ga flux stability, poor reproducibility, and no lasing devices. Two steps were taken to improve the THz structures: a switch to MBE configuration B along with the removal of Ga shutter operations, therefore no growth interrupts. This minimizes the flux variations for both thin layers and for long growths by using the dominant cell (Ga in this case) in steady state. The results are seen in the (002) XRD scan in Fig. 2. A 15 µm active region with 271 cascade periods is reproduced faithfully and what appear to be peak splitting, often seen in unstable long growths, are actually the diffraction peaks from the designed structure.

Table 1 summarizes the performance characteristics of the first four THz laser structures. The original 10-µm structure, 177 cascades, was designed to utilize both a surface plasmon and a double metal [5] waveguide by a 100 nm Al_{0.55}Ga_{0.45}As lift-off layer and 800 nm bottom contact layer. To reduce the waveguide losses from the double-metal cladding and contacts, the active region was increased 50% to 15 µm, 271 cascades, doping reduced to 1.25e16 cm^-3, and the bottom contact layer thickness was reduced to 100 nm. The GaAs-based QCL has a large advantage over other material
systems when growing 10-15 µm active regions because lattice matching is not a critical factor.

![Graph](image)

**Fig. 2:** X-ray diffraction (002) rocking curve of a 15 µm THz QCL active region with 271 cascade periods. The top (blue) curve is the measured scan and bottom (red) curve is the calculated diffraction pattern. What appear to be peak splitting are actually satellite peaks resulting from the designed structure.

**Table 1: Performance Characteristics of THz QCL with Decreasing Si Doping.**

<table>
<thead>
<tr>
<th>Waveguide</th>
<th>$J_{th}$ (kA/cm$^2$)</th>
<th>$T_{max}$ Pulsed</th>
<th>$T_{max}$ CW</th>
<th>Active Region</th>
<th>Doping (cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface Plasmon</td>
<td>1.88</td>
<td>88 K</td>
<td>-</td>
<td>10 µm</td>
<td>1.9e16</td>
</tr>
<tr>
<td>Double Metal</td>
<td>0.993</td>
<td>145 K</td>
<td>-</td>
<td>10 µm</td>
<td>1.9e16</td>
</tr>
<tr>
<td>Double Metal</td>
<td>0.506</td>
<td>145 K</td>
<td>25 K</td>
<td>15 µm</td>
<td>1.25e16</td>
</tr>
<tr>
<td>Double Metal</td>
<td>0.305</td>
<td>147 K</td>
<td>68 K</td>
<td>15 µm</td>
<td>8.0e15</td>
</tr>
<tr>
<td>Double Metal</td>
<td>0.205</td>
<td>133 K</td>
<td>72 K</td>
<td>15 µm</td>
<td>5.0e15</td>
</tr>
</tbody>
</table>

The double metal waveguide, due to strong mode confinement, resulted in a dramatic 50% reduction in $J_{th}$ and pulsed operation $T_{max}$. The first three samples lased up to 145 K with a characteristic $T_0$ of 33 K. However, the continuous wave (CW) operation of the three samples differed greatly, with CW up to 25 K only in the initial low doped structures. A further reduction in doping resulted in a lower $J_{th}$, increased CW $T_{max}$ of 72 K, at a cost of a reduction in the current operating range, output power, and pulsed $T_{max}$. 
Conclusion

A 15-µm active region terahertz (2.86 THz) quantum cascade laser was optimized for maximum continuous wave temperature operation. Through the use of high-resolution x-ray diffraction, improved growth rate and doping calibrations, minimization of flux transients, a double-metal waveguide, and optimization of doping the threshold current was reduced from 1.88 to 0.205 kA/cm² and a maximum continuous wave operating temperature of 72K was achieved. The tolerable thickness variation in one cascade period was <1.1%.

References