Optimization of semi-insulating surface-plasmon waveguides within terahertz QCL's using computational models

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Outline

• Introduction to quantum cascade lasers
• Mode solver and optimization algorithms
• Optimization of a 2.83 THz waveguide
• Optimum waveguides vs. frequency
• Many-layered waveguide optimization
• Optimization of a 3.43 THz waveguide
Introduction to QCL's

- compact source of coherent THz radiation
- security, medical, & scaled radar applications
- nanoscale semiconductor heterostructure
- low optical power limits use
- improving waveguide increases optical power
Semi-insulating Surface-plasmon waveguides

- metal on top, n+ GaAs on bottom, SI substrate
- mode penetrates deep into substrate
Mode Solver Algorithm

- slab waveguide model, one-dimensional in $x$
- only $x$-polarized TM modes excited:

$$E_{x,i}(x) = \frac{k_z}{\omega \varepsilon_i} H_{y,i}(x) \quad E_{z,i}(x) = \frac{i}{\omega \varepsilon_i} \frac{\partial}{\partial x} H_{y,i}(x)$$

- in each layer $i$, $H_y$ has the form:

$$H_{y,i}(x) = A_i e^{ik_{x,i}x} + B_i e^{-ik_{x,i}x} \quad \text{where} \quad k_{x,i} = \sqrt{\varepsilon_i \mu_i \omega^2 - k_z^2}$$

- $A_i$ and $B_i$ found by applying boundary conditions, finding complex $k_z$ that gives valid modes
Mode Solver Algorithm

figure of merit is the gain threshold $g_{\text{th}}$:

$$g_{\text{th}} = \frac{(\alpha_w + \alpha_M)}{\Gamma}$$

waveguide loss $\alpha_w = 2 \, \text{Im}(k_z)$

confinement factor $\Gamma = \frac{\int_{-\infty}^{\infty} |E_{x,i}(x)|^2 \, dx}{\int_{-\infty}^{\infty} |E_i(x)|^2 \, dx}$
Optimization Algorithm

- vary the doping and thickness of the contact layers to minimize $g_{th}$

- use an $n$-dimensional gradient descent method to find the minimum
Optimization Algorithm

1. Input initial structure
2. Choose near-by structures
3. MODE SOLVER
4. Calculate $g_\text{th}$ gradient
5. Advance structure along negative gradient
6. MODE SOLVER
7. Check if $g_\text{th}$ is decreasing
   - yes
   - no

8. Check convergence
   - no
   - yes

Output optimized structure
## Optimization of the Vitiello 2.83 THz QCL Waveguide

<table>
<thead>
<tr>
<th>Layer</th>
<th>Original Structure</th>
<th>Thickness (μm)</th>
<th>Doping (cm(^{-3}))</th>
<th>Optimized Structure</th>
<th>Thickness (μm)</th>
<th>Doping (cm(^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>metal</td>
<td>semi-infinite</td>
<td>-</td>
<td>-</td>
<td>semi-infinite</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>upper GaAs</td>
<td>0.08</td>
<td>5.0 × 10(^{18})</td>
<td></td>
<td>0.30</td>
<td>2.57 × 10(^{18})</td>
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</tr>
<tr>
<td>active region</td>
<td>11.61</td>
<td>4.4 × 10(^{15})</td>
<td></td>
<td>11.61</td>
<td>4.40 × 10(^{15})</td>
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<tr>
<td>lower GaAs</td>
<td>0.60</td>
<td>2.0 × 10(^{18})</td>
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<td>0.71</td>
<td>1.90 × 10(^{18})</td>
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<tr>
<td>substrate</td>
<td>semi-infinite</td>
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<td></td>
<td>semi-infinite</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
Optimization of the Vitiello 2.83 THz QCL Waveguide

Original

Optimized

\[ g_{th} = 45.9 \ \text{1/cm} \]

\[ g_{th} = 28.7 \ \text{1/cm} \]
Optimum Waveguides vs. Frequency

• Take traditional SISP structure

• Fix active region at typical width of 11.57 μm and typical doping of $3 \times 10^{15}$ cm$^{-3}$

• At each frequency, optimize width and doping of contact layers until $g_{th}$ is minimized
Widths and Dopings of Optimum Waveguides vs. Frequency

![Graph showing the relationship between frequency and waveguide dimensions. The graph illustrates the variations in widths and dopings across different frequency ranges for both upper and lower layers.]
Optimum Gain Threshold vs. Frequency

![Graph showing the relationship between gain threshold (1/cm) and frequency (THz). The graph indicates a decreasing trend as frequency increases.]
Many-Layered Waveguide Optimization

• Introduce more n+ layers between the bottom contact layer and the substrate
• Optimize these additional layers as well: may lower $g_{th}$ even more
• Difficulty 1: no unique solution
• Difficulty 2: multiple local minima
Many-Layered Waveguide Optimization
No Unique Solution

• When both widths and dopings are allowed to vary, endless combinations represent the same physical structure

• Answer: fix widths and vary only dopings
Many-Layered Waveguide Optimization
Multiple Local Minima

• Algorithm converges to different optimized waveguide structure with different $g_{th}$ for different initial structures = multiple local minima

• We want the best waveguide overall = global minimum

• Answer: Repeat algorithm many times until all local minima have been found, choose lowest
Optimization of a 3.43 THz QCL Many-Layered Waveguide

- 4 layers between active region and substrate
- Each lower layer fixed at 100 nm thick
- Optimize 81 times, global minimum obvious

![Graph showing the optimization process]
Optimization of a 3.43 THz QCL Many-Layered Waveguide

- original waveguide, $g_{th} = 23.8$ 1/cm
- normal layers optimized, $g_{th} = 21.2$ 1/cm
- many layers optimized, $g_{th} = 20.3$ 1/cm
Conclusions

• Systematic optimization of QCL SI-SP waveguide layer widths and dopings can yield significant performance improvement.
• QCL's below 2 THz can successfully use SI-SP waveguides if optimized properly.
• Insertion and optimization of additional lower n+ layers may further improve waveguide performance.

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