Simulation study in Design of Miniaturized Mid-Infrared Sensors

X. Wang, S-S. Kim, B. Mizaikoff*
→ MIR sensors combined with quantum cascade lasers (QCL)

→ MIR GaAs/Al$_{0.2}$Ga$_{0.8}$As waveguides
  Strip waveguides
  Slot waveguides

→ Simulation studies on MIR waveguide design
Quantum Cascade Lasers (QCL)

1994 - Breakthrough in IR light source technology

- Layers of semiconductor materials create a quantum heterostructure
- Common materials are: InGaAs/AlInAs/InP and GaAs/AlGaAs

- Photons produced by intersubband transitions rather than recombination processes
- Layer dimensions dictate energy levels in heterostructure (quantum wells)
- Cascaded structures may produce multiple photons per electron

MIR Waveguide Design

Metal-organic vapor phase epitaxy (MOVPE)

**Growth parameters**
- MOVPE AIX – 200
- Materials used: TMGa, TEGa, TMAI, AsH$_3$,
- Horizontal reactor at 100 mbar
- $T_G = 750^\circ$ C

**Process flow**

Dr. Boris Mizaikoff
boris.mizaikoff@uni-ulm.de
MIR Waveguides

Towards superior mode control with GaAs/Al$_{0.2}$Ga$_{0.8}$As waveguides

- Frequency matched to QCL emission
- Well-defined evanescent field
- Superior mode control
- Toward the theoretical sensitivity limits of evanescent field sensing
Chip-integrated IR devices

→ Strip waveguide microfabrication via RIE (reactive ion etching)

→ 200/100/50... µm wide waveguide strips

→ QCL emission at 974 cm\(^{-1}\) overlaps with absorption of analyte (acetic anhydride)
Sing Mode laser of EC-QCL

Mode analysis of EC-QCL with MIR camera

→ Wavenumber: 1665 cm\(^{-1}\)
→ Duty cycle: 1%
→ Repetition rate: 100 kHz
→ Evidence of single mode pulse lasing of the EC-QCL (1575-1735 cm\(^{-1}\))
QCL Combined with Strip Waveguides

Calibration of coverage length

Measurements with strip waveguides

→ Analyte: acetic anhydride
→ 200 µm wide waveguide
→ Micro-capillary used to generate 2 nL droplets
→ pseudo Lambert-Beer law:

\[ A = (\epsilon \times c \times l) r \]

EW ratio: \( r = \frac{I_e}{I_0} \)

(I_e: evanescent filed intensity, I_0: total intensity of guided light)

System response for GaAs strip waveguide as a function of the coverage length with linear fit. Each 2 nL droplet covered a diameter of 0.4 mm.
QCL Combined with Strip Waveguides

Calibration of concentration

System response to diluted acetic anhydride in diethylene glycol monoethyl ether. Each 2 nL droplet covered a diameter of 0.4 mm.

Measurements with strip waveguides

→ Analyte: acetic anhydride
→ 200 µm wide waveguide
→ Micro-capillary used to generate 2 nL droplets
→ pseudo Lambert-Beer law:
  \[ A = (\varepsilon \times c \times l) r \]

EW ratio: \( r = \frac{I_e}{I_0} \)
(\( I_e \): evanescent filed intensity, \( I_0 \): total intensity of guided light)
QCL Combined with Strip Waveguides

Comparison strip waveguide vs. slab waveguide

Strip waveguide vs. slab waveguide

→ CH$_3$-C bending vibration of acetic anhydride overlap with QCL emission
→ LOD of 0.2 pL (2 pmol)
→ One order of magnitude improvement vs. slab waveguide
→ Further improved sensitivity anticipated via narrowing strip width
Mode Analysis of GaAs/Al$_{0.2}$Ga$_{0.8}$As with COMSOL

Single Mode Waveguides

RF module, Electromagnetic Waves (emw).

Geometry and Material parameters:
Core: 6 um GaAs, n=3.3
Cladding: 6 um Al$_{0.2}$Ga$_{0.8}$As, n=3.2
Wafer: GaAs (doped), n= 3.2
Air: n=1
Width of WG: 5 um
Wavelength: 6.01 um (1665 cm$^{-1}$)
Single Mode: TEM (0.0)
2D mode analysis with strip width of 5 µm
Red line stands for the cross-section in y-axis
Red arrow stands for the direction of electrical field: $E_x$ along x-axis.

Intensity Fraction of evanescent field over the total beam is calculated to be 0.06 % along the cross-section.

$E_x$ distribution along the cross-section with effective mode index of $n_{\text{eff}} = 3.22$.
Mode Analysis of GaAs/Al$_{0.2}$Ga$_{0.8}$As

The penetration depth $D_p$ of evanescent field is estimated to be 1 µm in the simulation. The fraction of evanescent field is calculated to be 0.3 % for each interface along the cross-section.

$E_x$ distribution with $n_{eff} = 3.22$. There is discontinuity of $E_x$ on interface between the core and air ($x = 3.5, 8.5$).
$E_y$ distribution along the line is analyzed in the diagram on the right ($n_{eff1}=3.22948$). There is discontinuity of $E_y$ on interface of vacuum and the core ($x=2$ um).
$E_y$ distribution along the line is analyzed in the diagram on the right ($n_{eff1}=3.22948$). There is no discontinuity of $E_y$ on interface of vacuum and the core ($x=3.5$ and $8.5$). The penetration depth $D_p$ of evanescent field is around $1 \text{ um}$.
The $E_y (0, 0)$ behaves as an exponential curve and the EW ratio achieves $r_e > 1\%$ with cutoff width $D_c = 4\, \text{um}$ at $1665\, \text{cm}^{-1}$. 

Reference

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MIR Slot Waveguides

Advanced waveguide design with FEM simulations

SlotStrip waveguide vs. strip waveguide
- WG width: 10 µm
- Trench width: 200 / 600 nm

→ pseudo Lambert-Beer law:
\[ A = (\varepsilon c l) r \]

→ EW ratio: \( r = \frac{l_e}{l_0} \)
(\( l_e \): evanescent filed intensity, \( l_0 \): total intensity of guided light)

→ Enhancement factor: up to 1-2 orders of magnitude expected!

Dr. Boris Mizaikoff
boris.mizaikoff@uni-ulm.de
Conclusions and Outlooks

→ Simulation studies on GaAs/AlGaAs strip waveguide

→ Optimization of single mode MIR strip waveguide
  Simulation & experiment

→ 3-D Simulation of beam propagation in strip waveguide

→ Resonator based waveguide design
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The Electromagnetic Waves interface, analyzes frequency domain electromagnetic waves, and uses time-harmonic and eigenfrequency/eigenmode studies.

**It Provides:**

- Flexible what-if-scenarios
- Physics Solution
- Solving Equations

**Work process:**

1. Model Meshing
2. Applicate of material properties
3. Add the Physics
4. Defining the boundary conditions
5. Compute

**Maxwell Equations**

- Divergence equations
- Curl equations

**Electric:**
\[ \nabla \cdot \mathbf{D} = \rho \]
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]

**Magnetic:**
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \]

**Wave Equations**

**Electric:**

**Magnetic:**

Reference: www.comsol.com

Dr. Boris Mizaikoff
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Waveguide structure: Slab waveguide (WG)
Polarization: TM
Mode index: $m = 0$
Refractive Index of GaAs: $n_1 = 3.3$
Refractive Index of air: $n_2 = 1$

Slab waveguide with symmetric structure does not own cut-off thickness. Penetration depth $D_p$ show dramatical increase as thickness of waveguide narrows down to sub-wavelength range.
Cutoff width $D_c$ of strip WG at 1665 cm$^{-1}$ are 4.5 um for $E_y$ and 5 um for $E_x$ TE (0,0) mode respectively.

Effective mode index $n_{\text{eff}}$ must fulfill the range: $n_l > n_{\text{eff}} > n_c$

As strip narrows down to $D_c$, $n_{\text{eff}}$ approach to $n_c$. 

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The strip waveguide will support higher order modes of light as \( w \) increases.

According to the simulation results from the diagram on the left, in order to avoid the generation of higher order modes of light, the width should be confined within 8 \( \mu \text{m} \) (\( D_c \) in \( E_x(1.0) \) mode).