COMSOL CONFERENCE
STUTTGART
2011

Simulation study in Design of Miniaturized Mid-Infrared Sensors

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Stuttgart, 10/27/11, 11:00 am.

Content

→ 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

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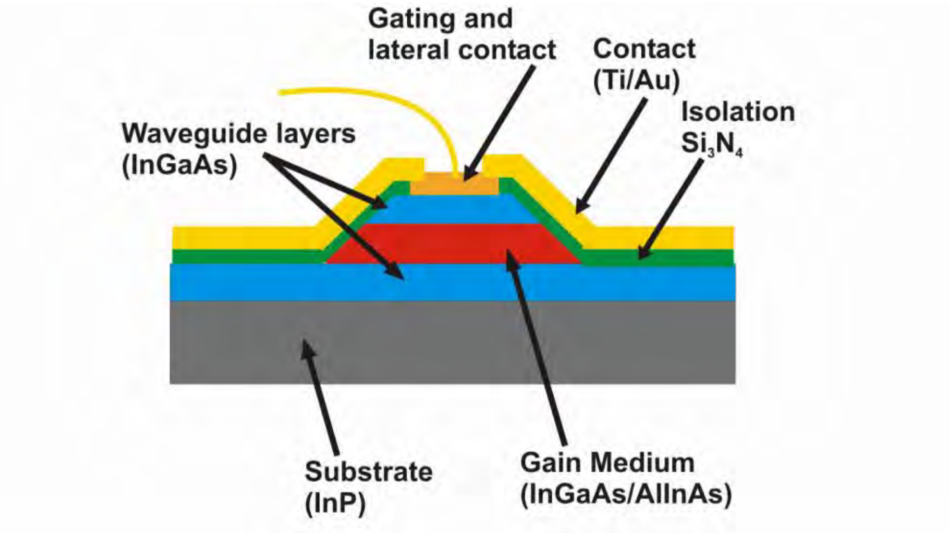
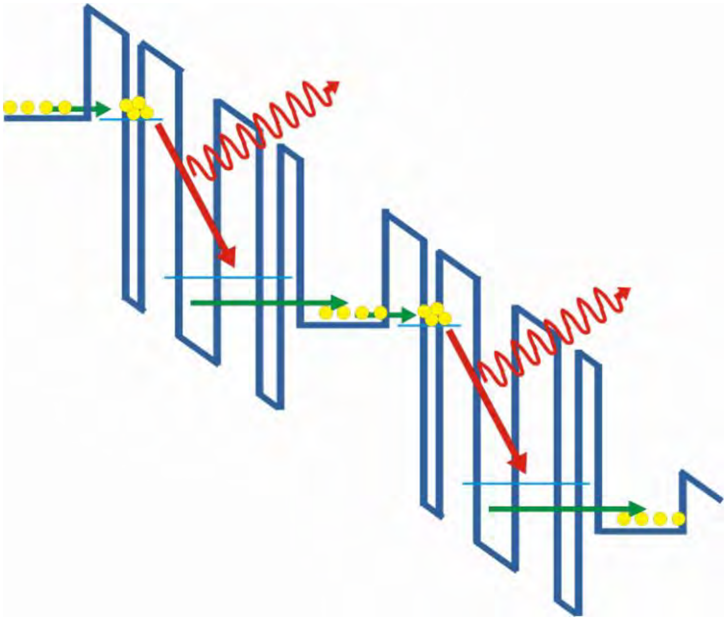
Quantum Cascade Lasers (QCL)

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

J.Faist, et al., Science, 264, 553 (1994)

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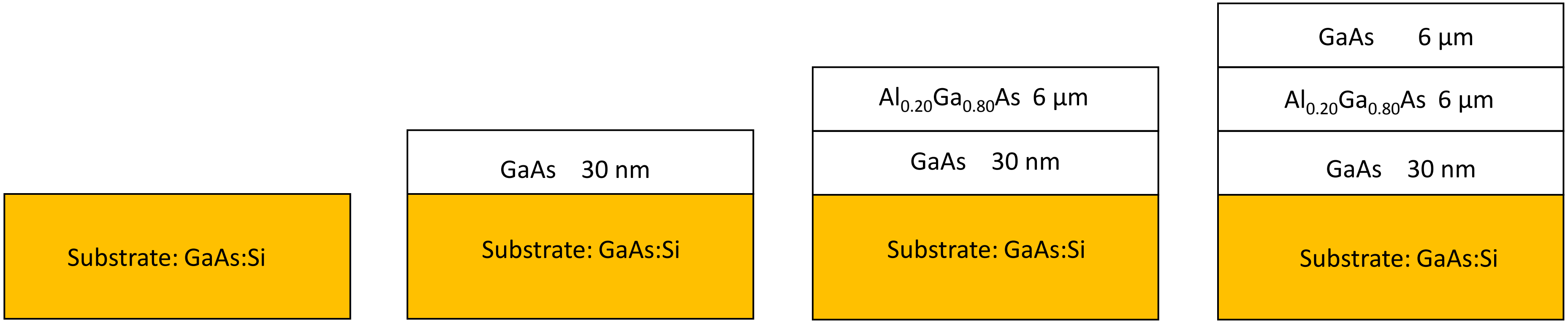
MIR Waveguide Design

Metal-organic vapor phase epitaxy (MOVPE)

Growth parameters

- MOVPE AIX – 200
- Materials used:
  TMGa, TEGa, TMAl, AsH_3,
- Horizontal reactor at 100 mbar
- $T_G = 750^\circ$ C



Process flow

S.-S. Kim, et., Anal. Bioanal. Chem.390, 231 (2008)

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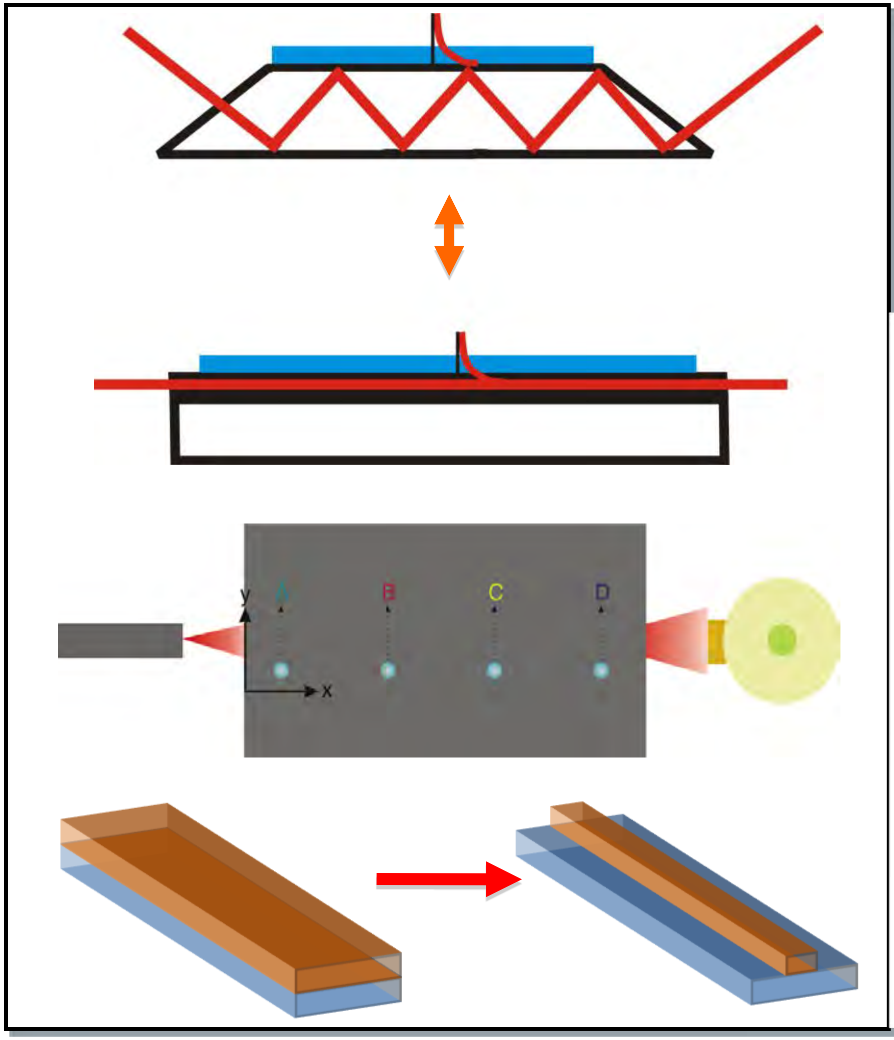
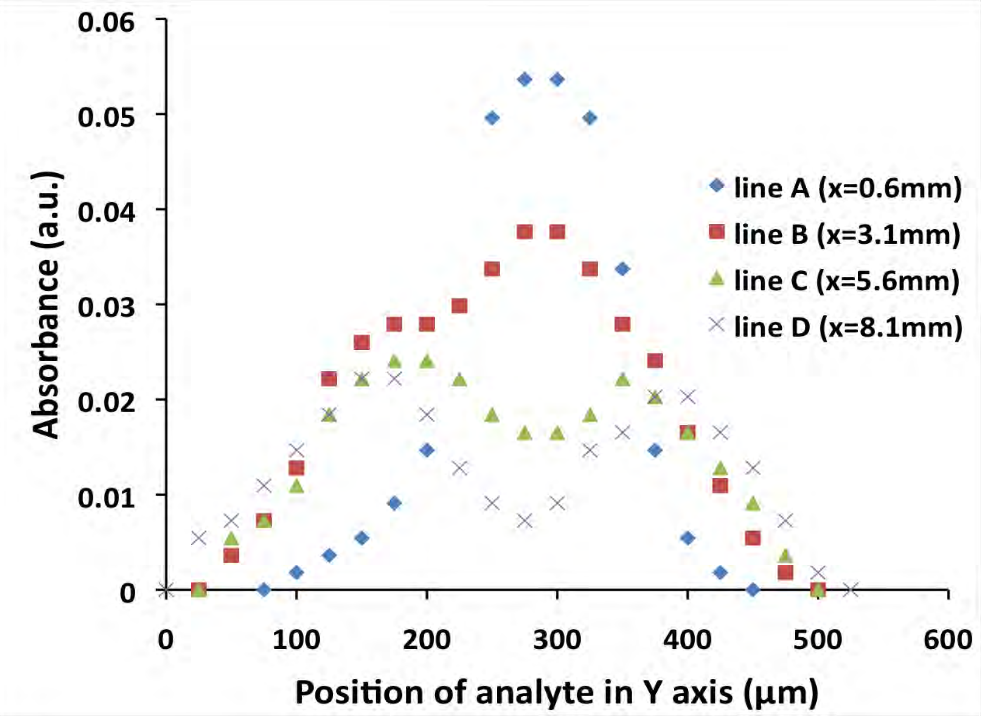
MIR Waveguides

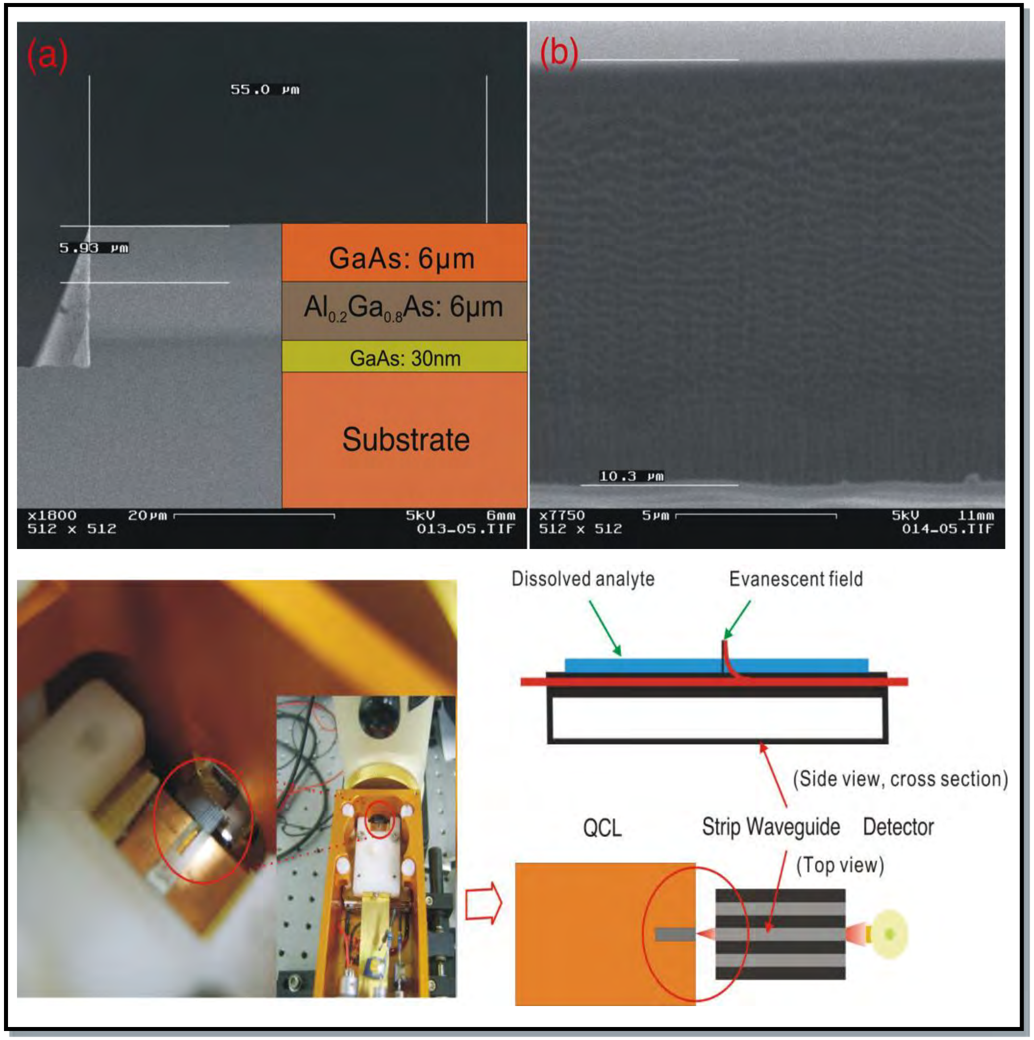
Towards superior mode control with GaAs/$Al_{0.2}Ga_{0.8}As$ waveguides



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



QCL Combinded with Strip Waveguides



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)

C. Charlton, et., Anal. Chem. 78, 4224 (2006)

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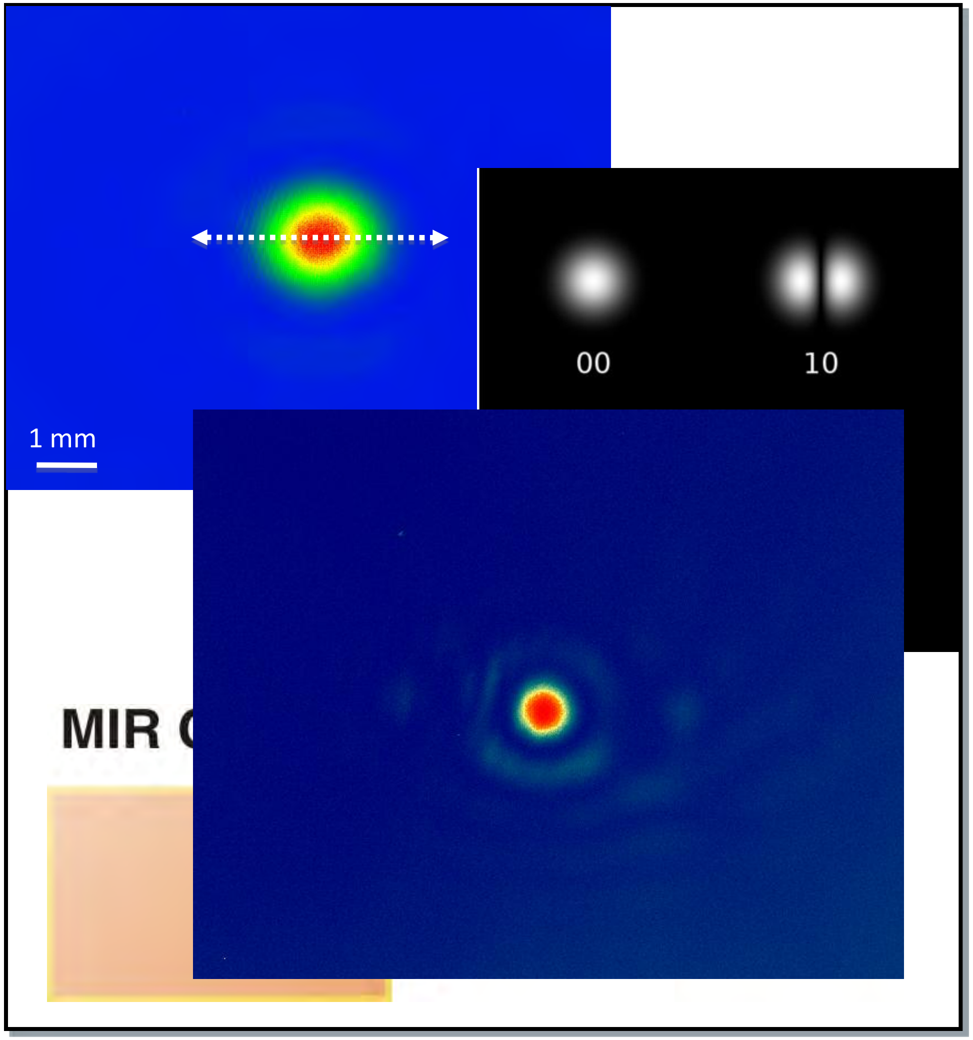
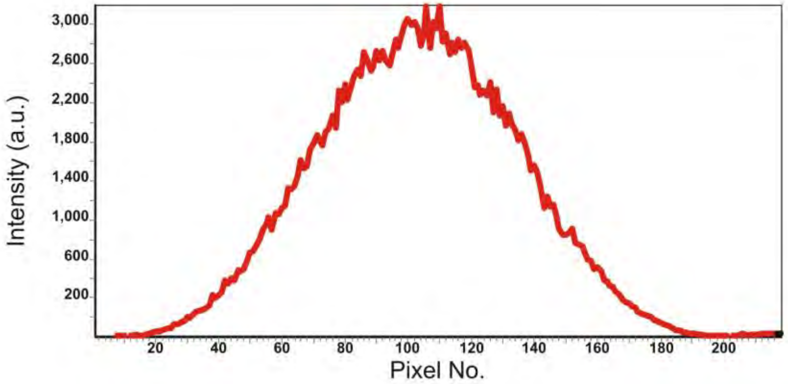
Sing Mode laser of EC-QCL

Mode analysis of EC-QCL with MIR camera



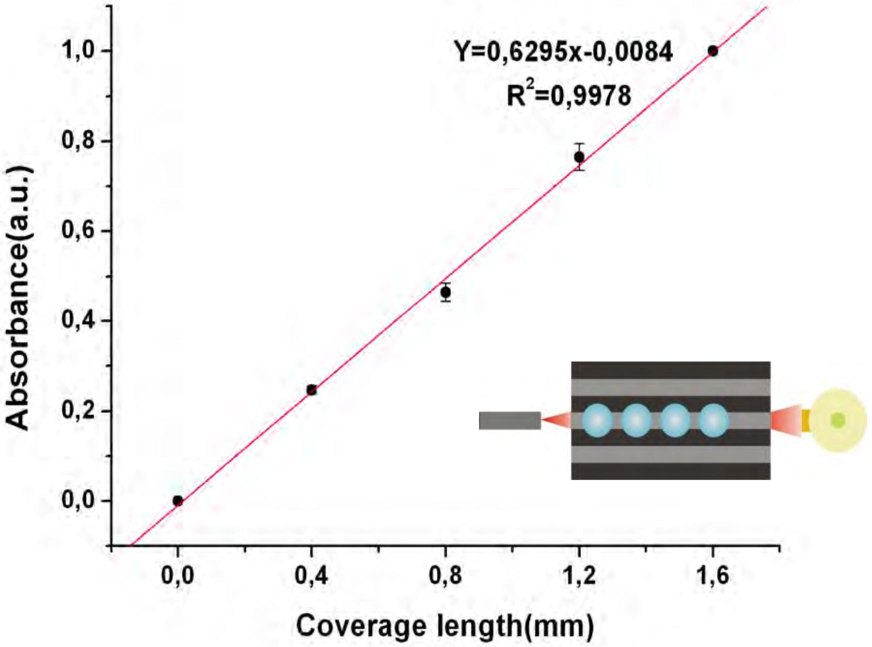
Beam Profile of EC-QCL in pulse mode

→ 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



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.

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: $r = I_e/I_0$
(I_e : evanescent filed intensity, I_0 : total intensity of guided light)

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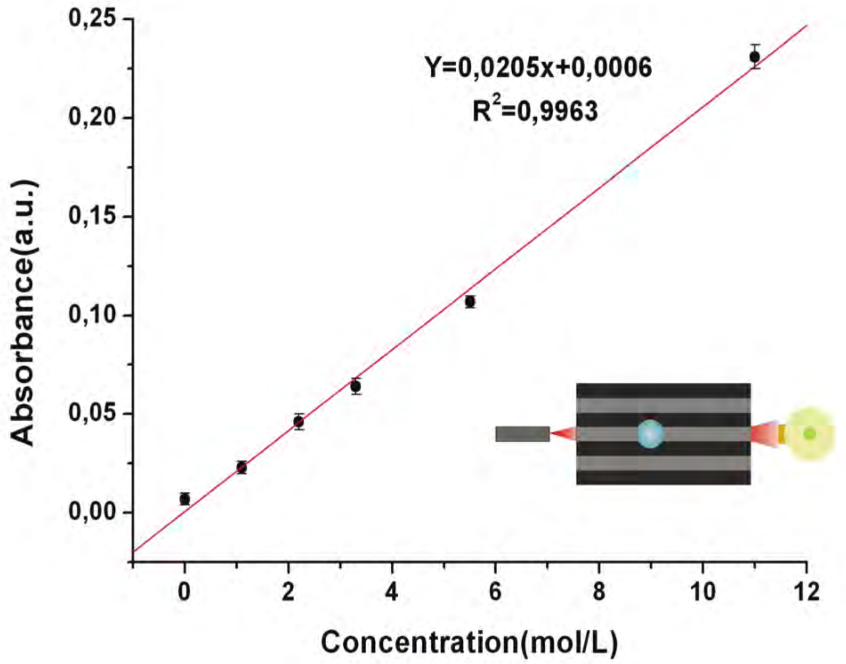
QCL Combined with Strip Waveguides

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:

$$\mathbf{A = (\varepsilon \times c \times l)\, r}$$

EW ratio: $r = I_e/I_0$
(I_e : evanescent filed intensity, I_0 : total intensity of guided light)

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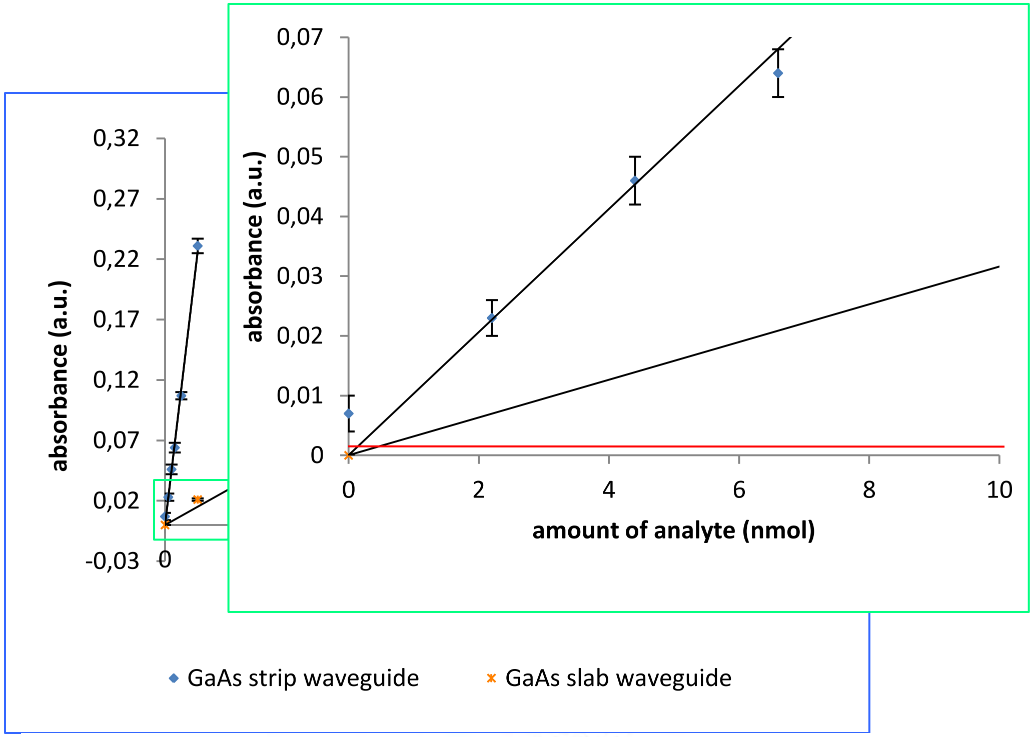
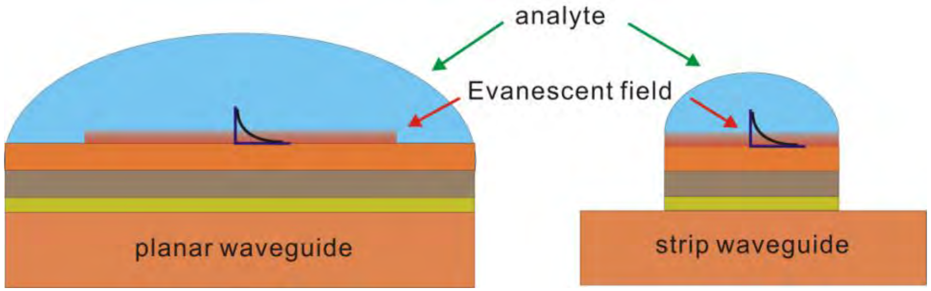
QCL Combined with Strip Waveguides

Comparison strip waveguide vs. slab waveguide





Strip waveguide vs. slab waveguide

→ CH_3-C bending vibration of acetic anhydride overlap with QCL emission

→ 200 µm wide waveguide

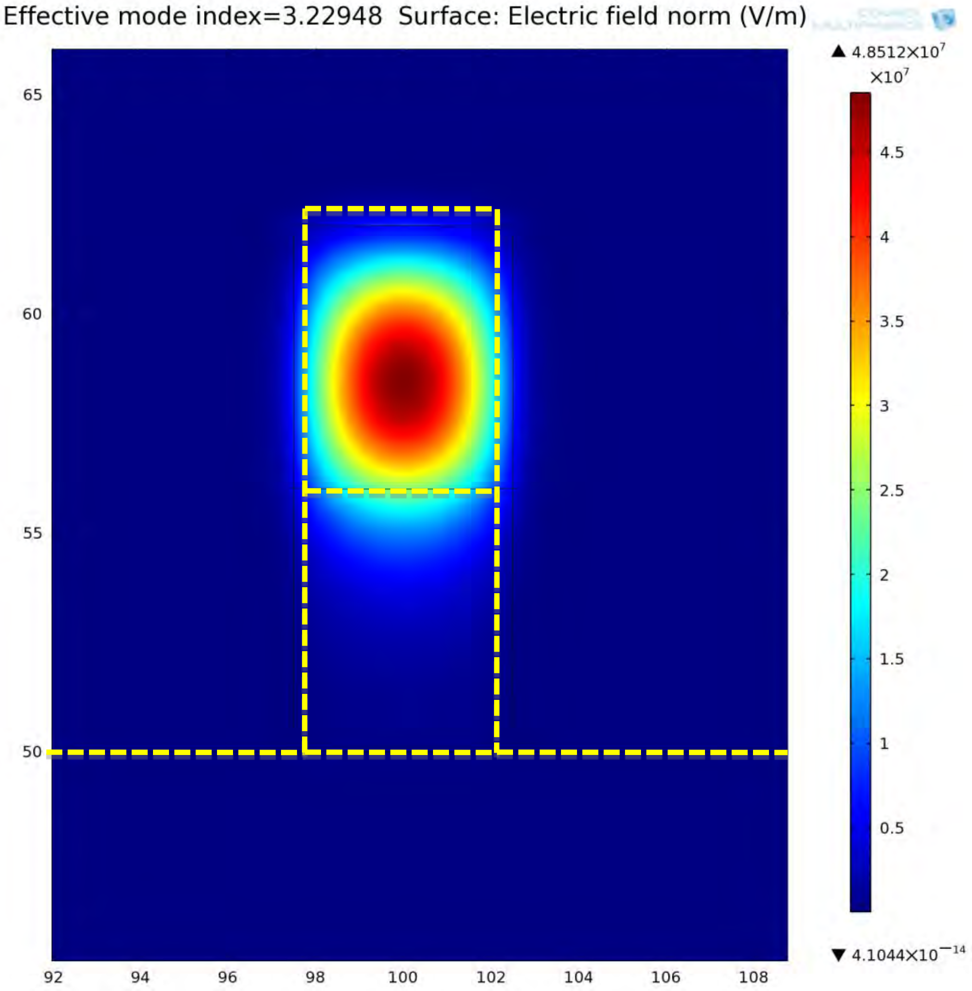
→ **LOD of 0.2 pL (2 pmol)**

→ 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
Clading: 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)

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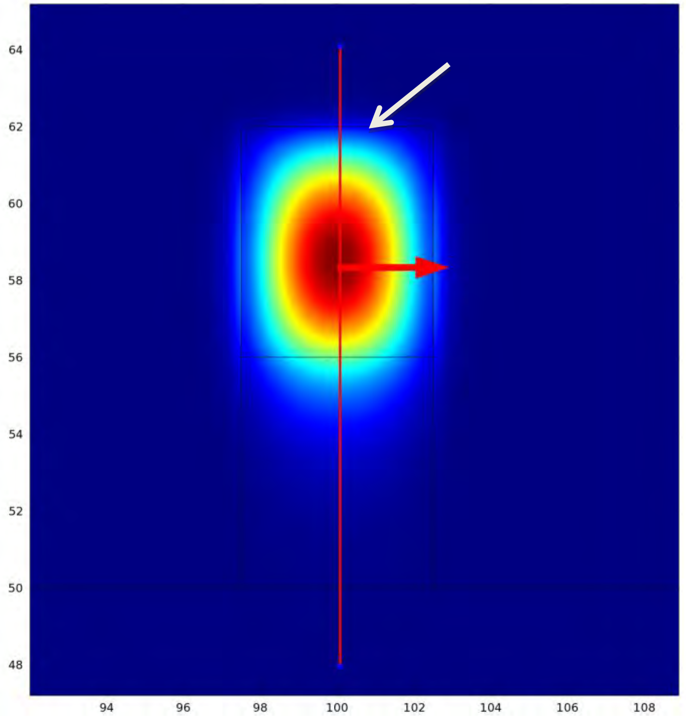
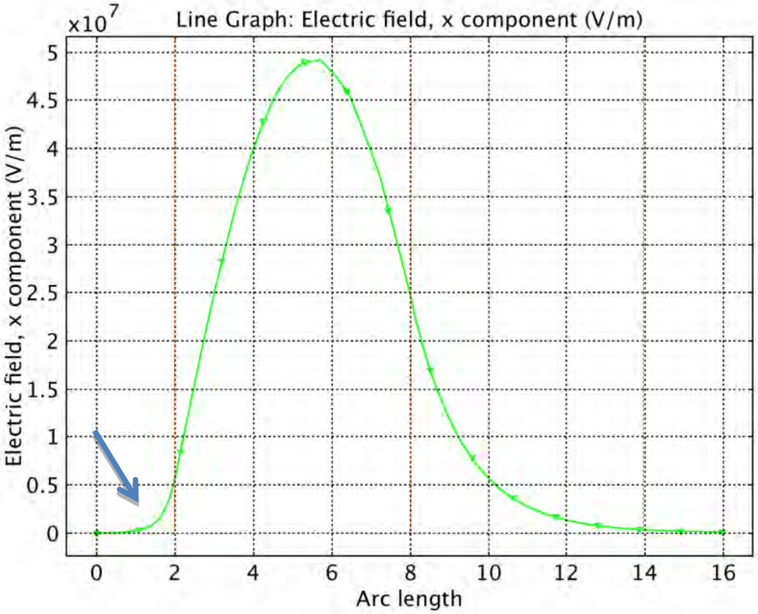
Mode Analysis of GaAs/$Al_{0.2}Ga_{0.8}As$





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.

E_x distribution along the cross-section with effective mode index of n_{eff} = 3.22.
Acr length (0 - 2): evanescent field, (2 - 8): core, (8 - 14): clading, (14 - 16): substrate.

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

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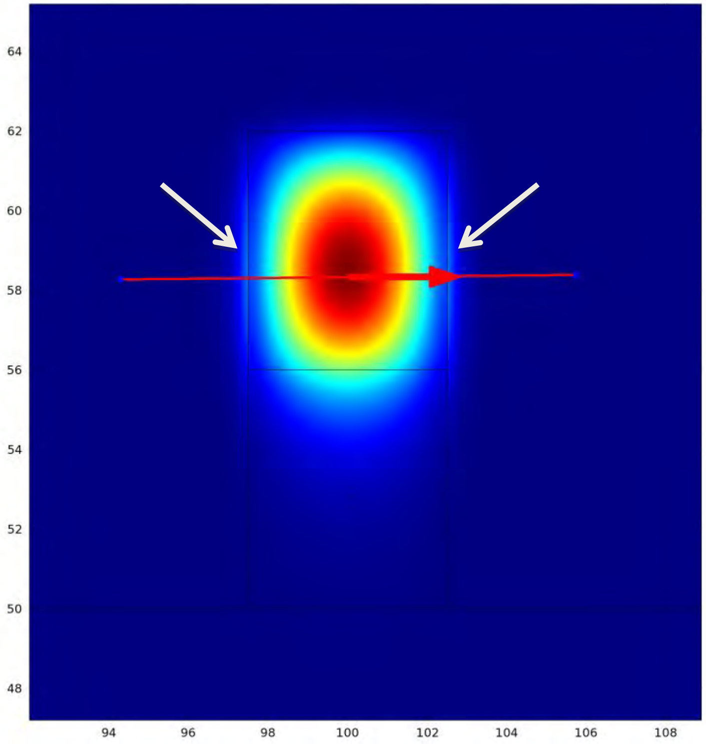
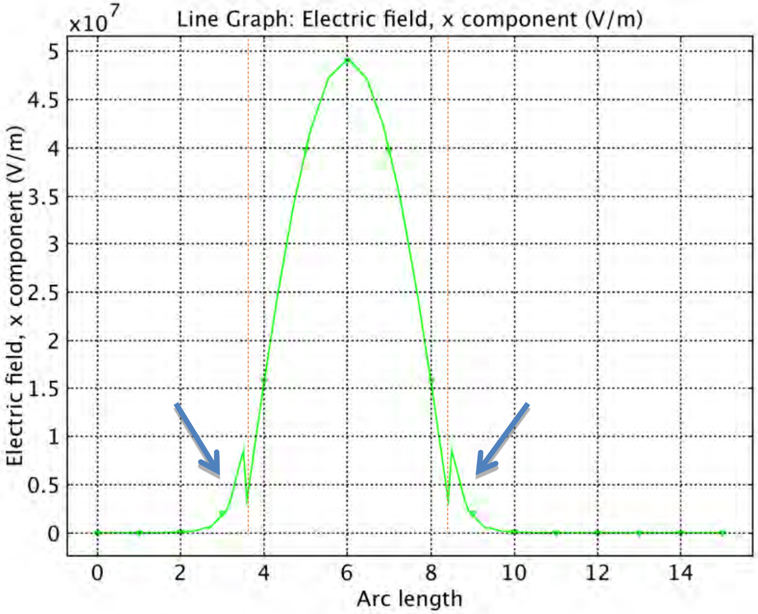
Mode Analysis of GaAs/$Al_{0.2}Ga_{0.8}As$

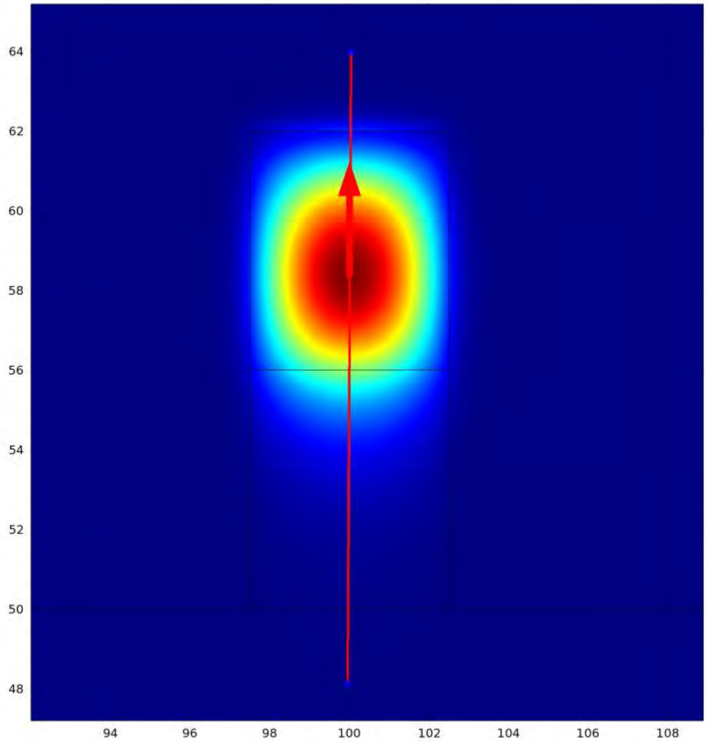


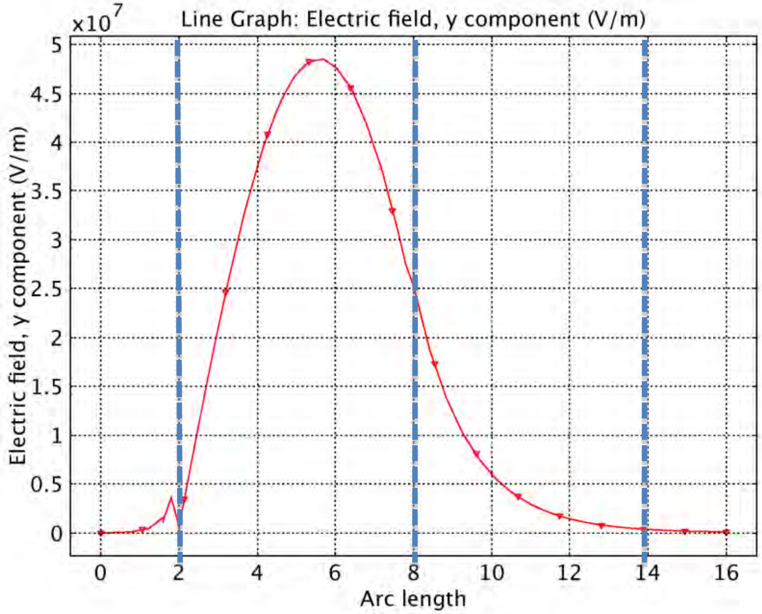


E_x distribution with n_{eff} = 3.22. There is discontinuity of E_x on interface between the core and air (x = 3.5, 8.5).

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.

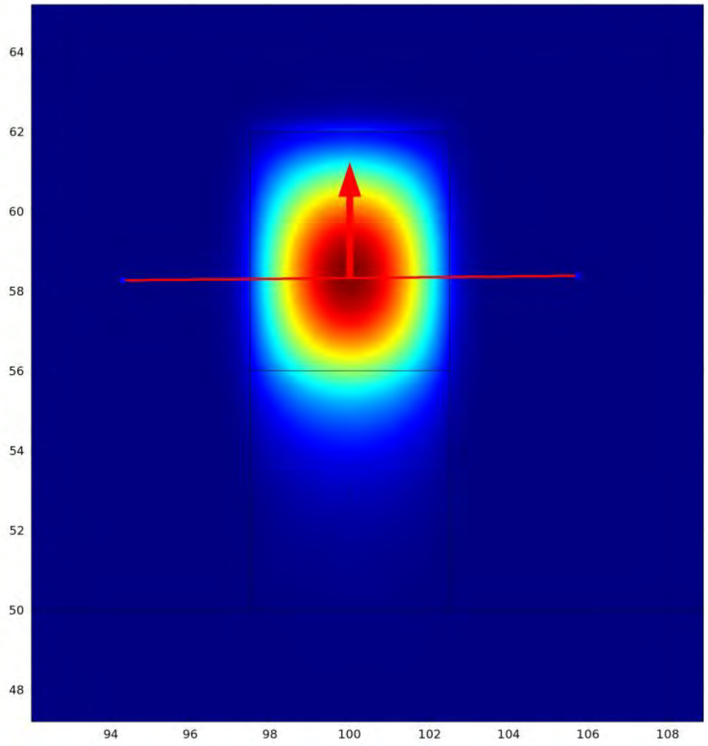
Mode Analysis of $GaAs/Al_{0.2}Ga_{0.8}As$ with COMSOL

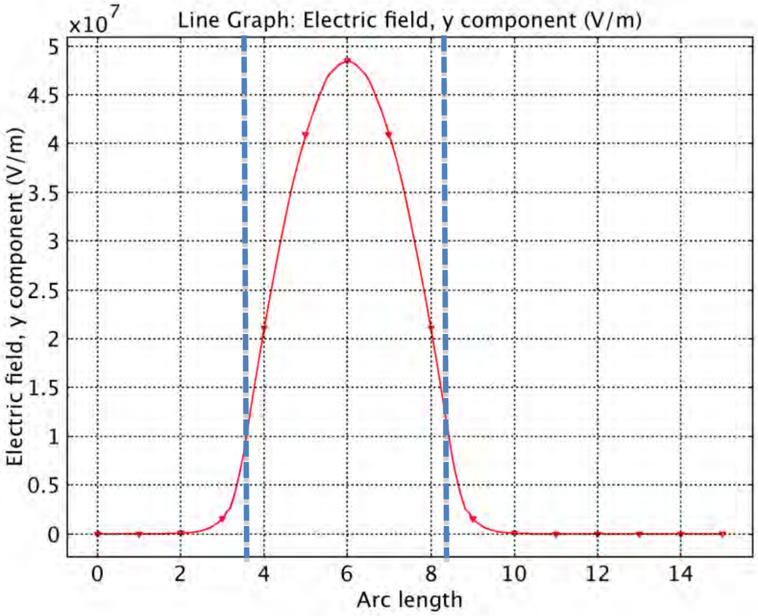




E_y distribution along the line is analyzed in the diagram on the right (n_{eff1}=3.22948). There is discontinuity of E_y on interface of vacuum and the core (x=2 um).

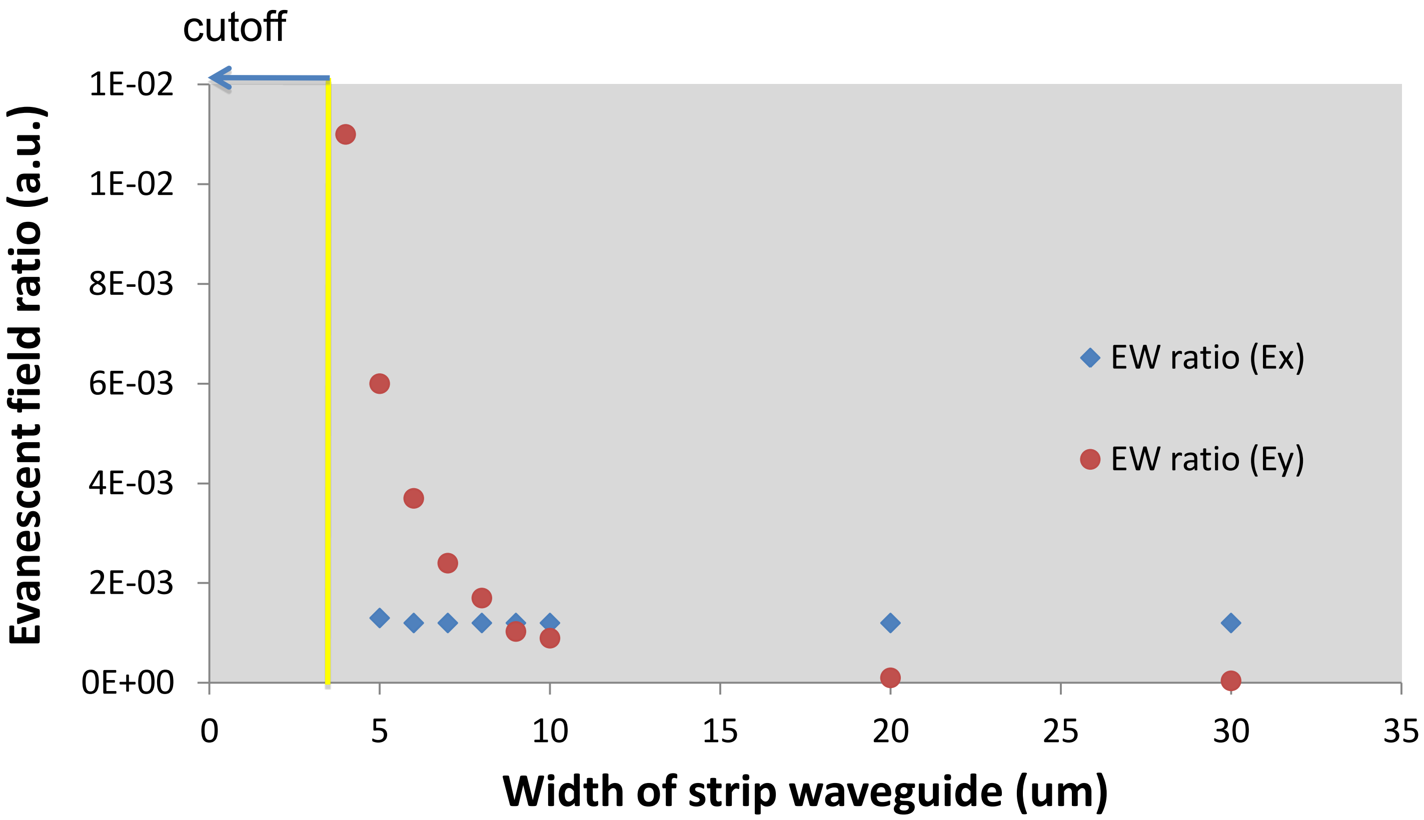
Mode Analysis of GaAs/$Al_{0.2}Ga_{0.8}As$ with COMSOL





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 um.

Mode Analysis of GaAs/$Al_{0.2}Ga_{0.8}As$



The E_y (0, 0) behaves as an exponential curve and the EW ratio achieves $r_e > 1$ % with cutoff width $D_c = 4$ um at 1665 cm^{-1}.

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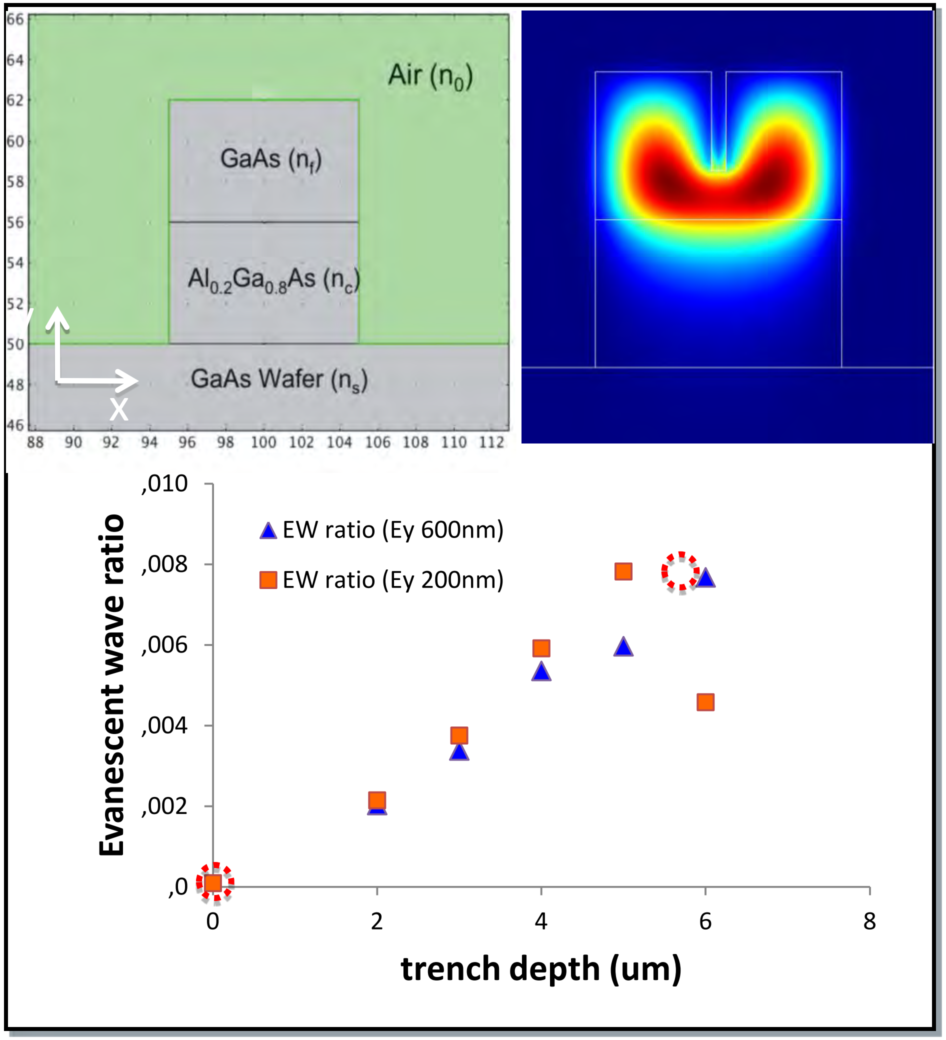
MIR Slot Waveguides

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 = (εcl) r

→ EW ratio: $r = I_e/I_0$

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

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

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Conclustions 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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Dr. C. Kranz

Thanks for your attention!

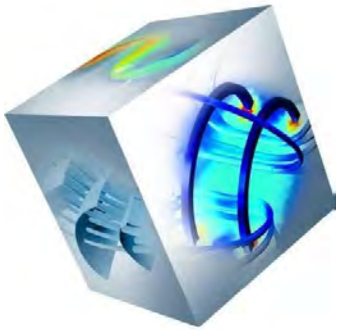
Simulation Study

COMSOL – RF-Module

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

It Provides:

Flexible what-if-scenarios 1.
Physics Solution 2.
Solving Equations 3.



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:	$\nabla \cdot \boldsymbol{D} = \rho$	$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$
Magnetic:	$\nabla \cdot \boldsymbol{B} = 0$	$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}$

$\boldsymbol{D}$ = Electric flux density
$\boldsymbol{E}$ = Electric field vector
ρ = charge density

$\boldsymbol{B}$ = Magnetic flux density
$\boldsymbol{H}$ = Magnetic field vector
$\boldsymbol{J}$ = current density

Wave Equations

Electric: [illegible]

Magnetic: [illegible]

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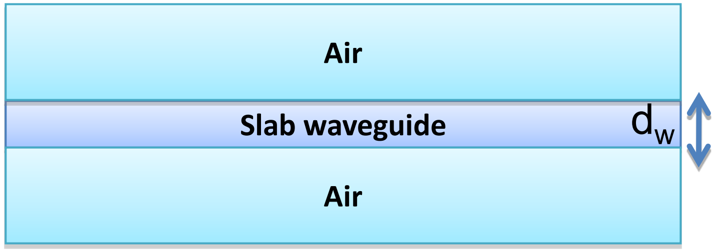
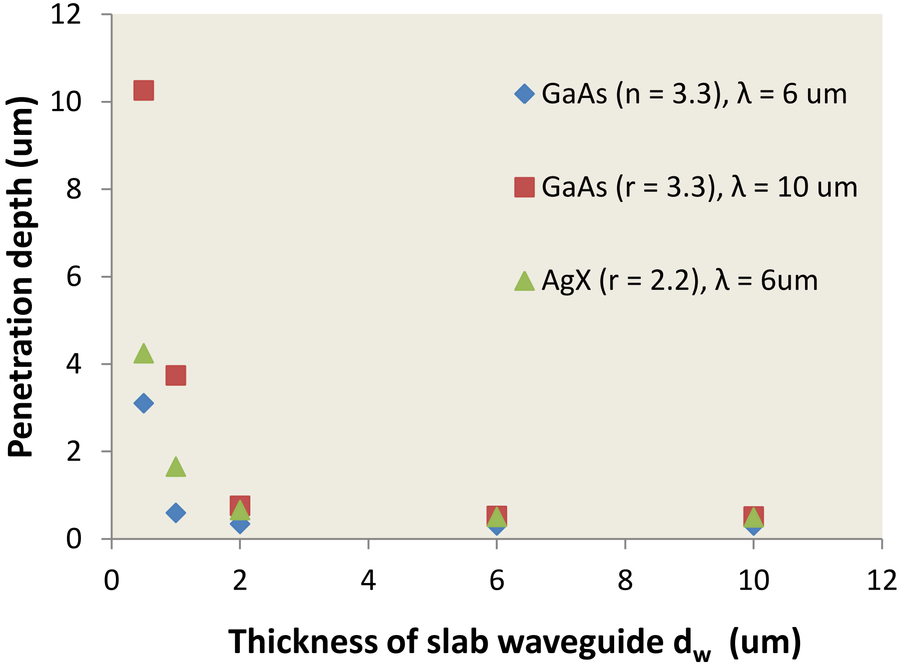
Mode Analysis of GaAs/$Al_{0.2}Ga_{0.8}As$ with COMSOL





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.

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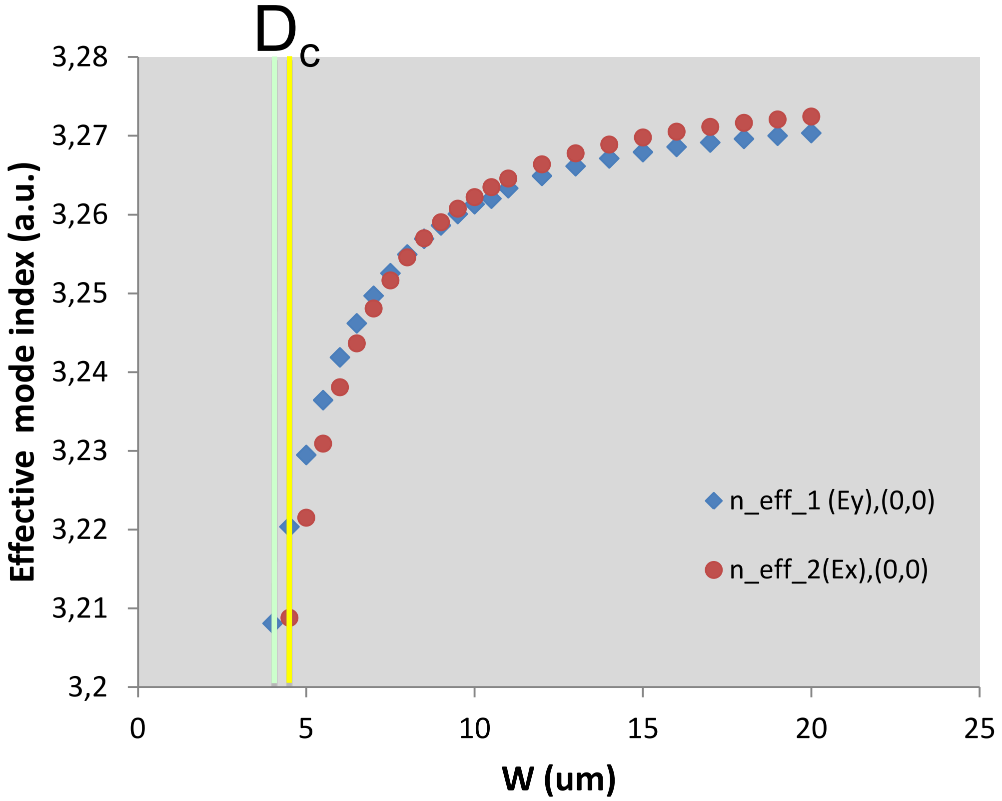
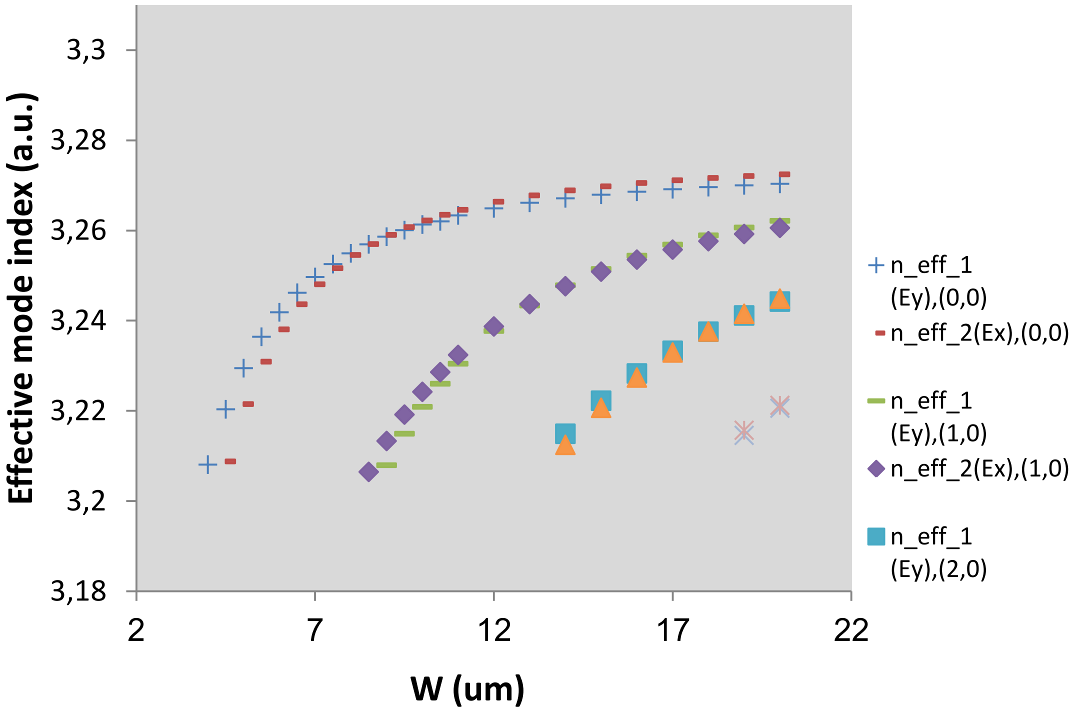


Cutoff width D_c of strip WG at 1665 cm^{-1} are 4.5 um for E_y and 5 um for E_x TE (0,0) mode respectively.

Effective mode index n_{eff} must fulfill the range: $n_f > n_{eff} > n_c$

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

Mode Analysis of GaAs/Al$_{0.2}$Ga$_{0.8}$As with COMSOL



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 um (D$_c$ in E$_x$(1.0) mode).