SIEMENS

FEM Simulations of Rod-Type Photonic Crystal Slabs as Resonant Microsystems for Optical Gas Sensors

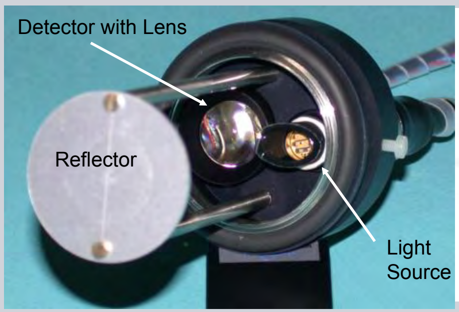
M.Sc. Christian Kraeh and Dr. Harry Hedler
Siemens AG, Corporate Technology

Excerpt from the Proceedings of the 2011 COMSOL Conference in Stuttgart

Motivation: From a conventional gas sensor to a small integrated gas sensor

SIEMENS

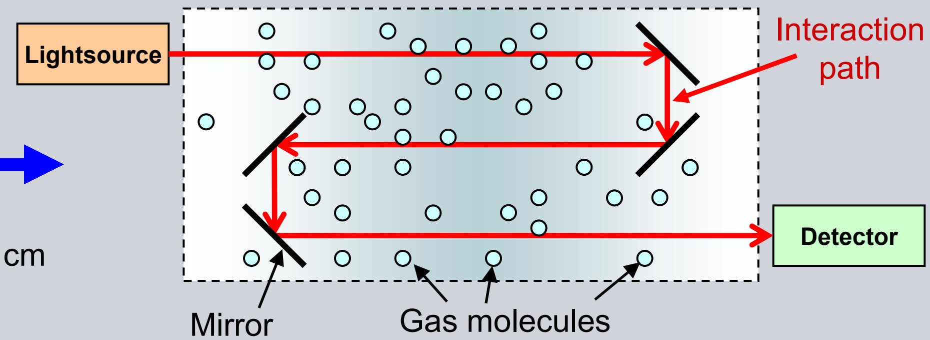
Gas detection with IR spectroscopy

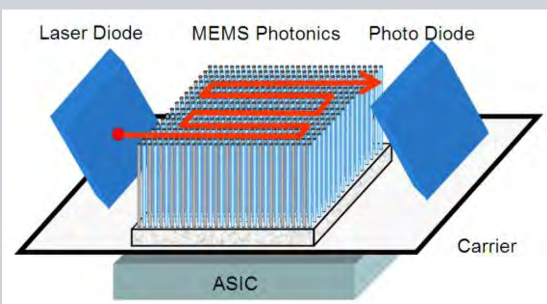


Conventional design

Size:
10 – 100 cm

Conventional spectroscopic gas sensor:

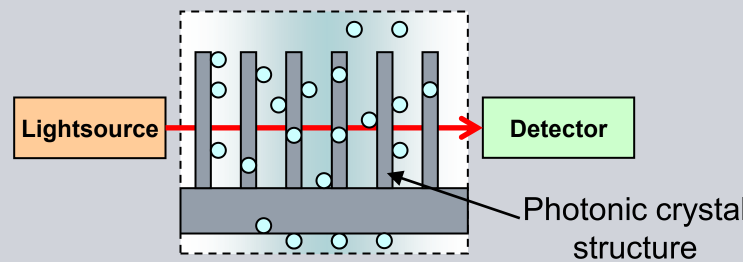




Small integrated sensor

Size:
0.1 – 1 cm

Photonic Crystal based gas sensor:



We used COMSOL Multiphysics to simulate light propagation in the photonic crystal

Outline

Photonic crystal structures

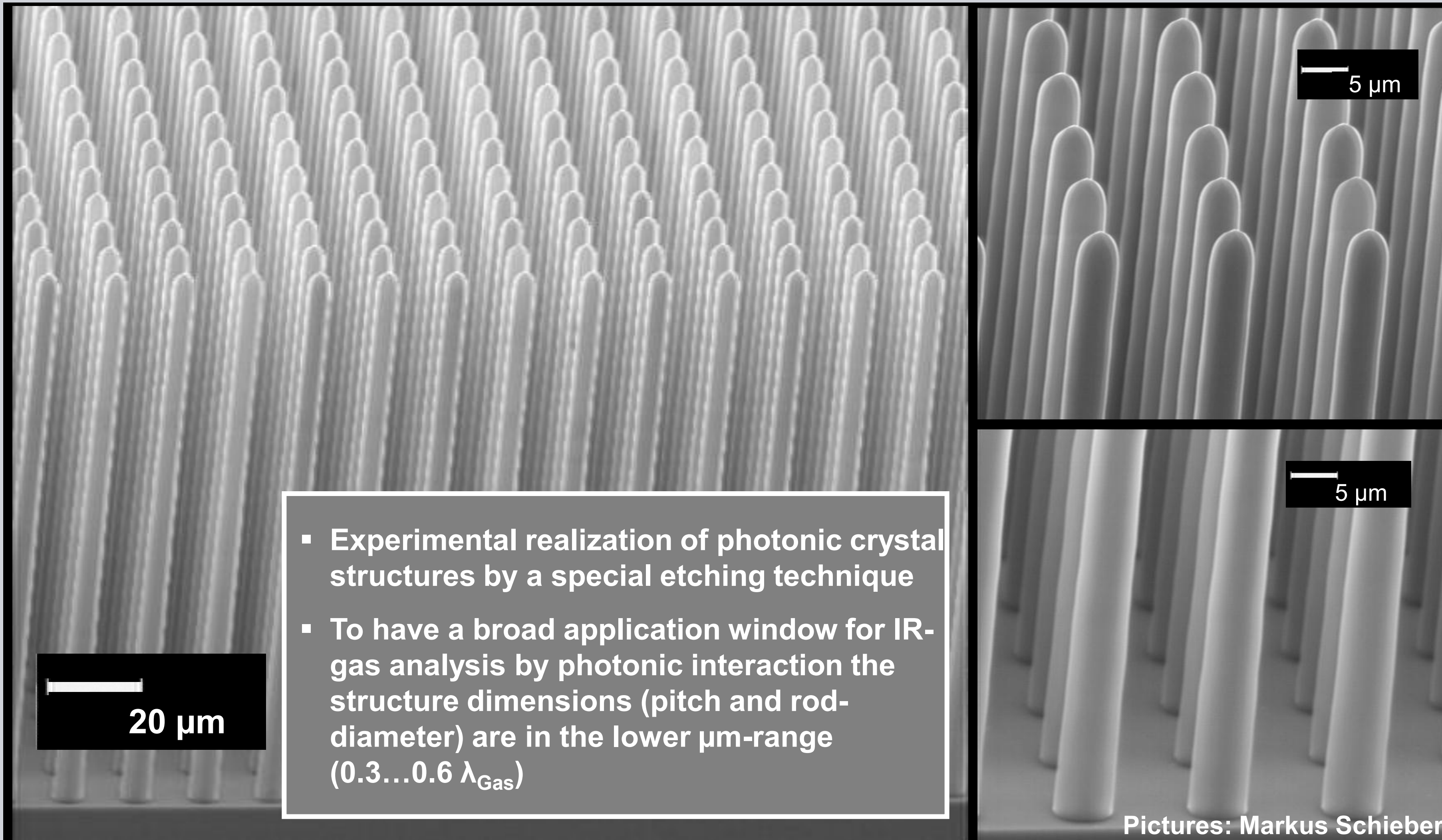
Simulations with COMSOL Multiphysics

- Optical properties of a photonic crystal
- Photonic crystal waveguides
  - Slow light for gas detection
  - Coupling into photonic crystal waveguides
- Simulation of the gas detection

Conclusion

SIEMENS

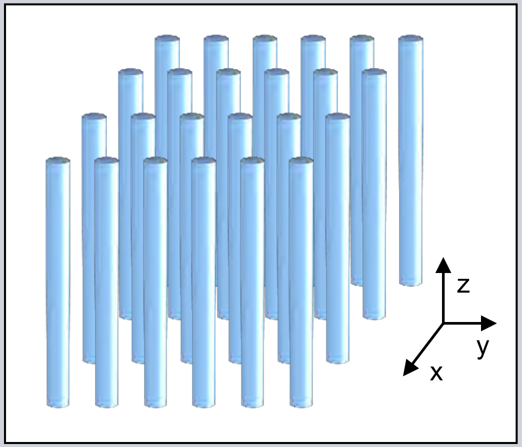
Photonic crystal structures



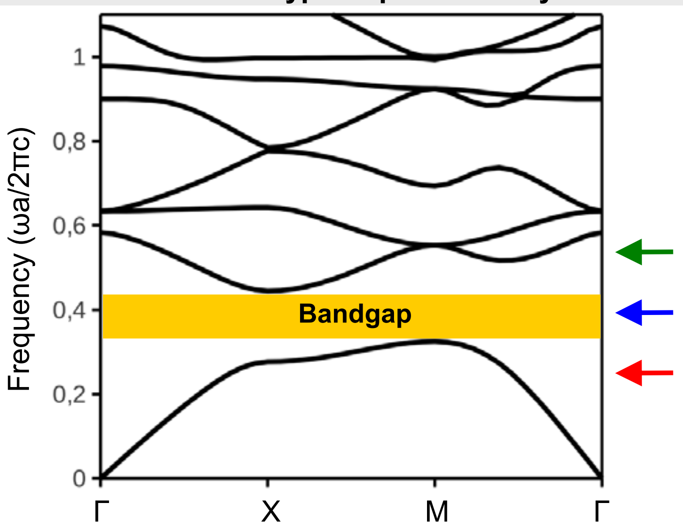
- **Experimental realization of photonic crystal structures by a special etching technique**
- **To have a broad application window for IR-gas analysis by photonic interaction the structure dimensions (pitch and rod-diameter) are in the lower µm-range (0.3…0.6 λ_{Gas})**

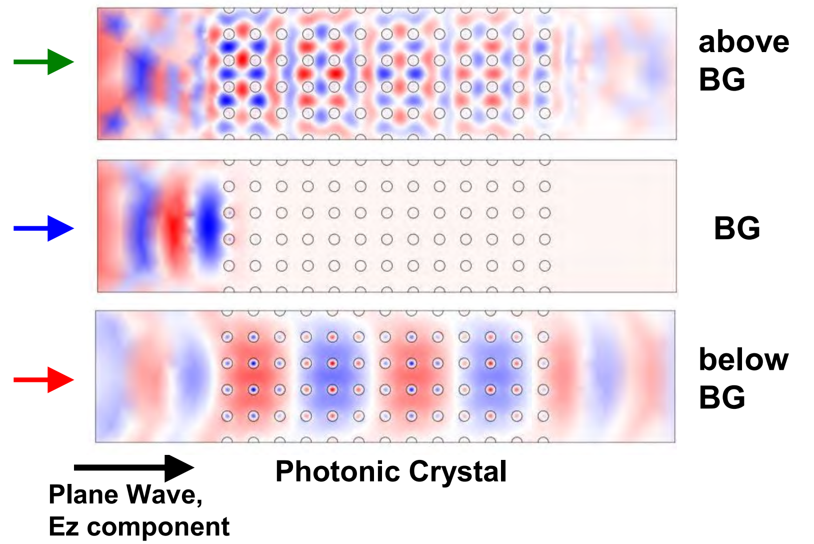
Optical properties of a photonic crystal

- Photonic crystals are composed of periodic dielectric structures that affect the propagation of EM waves
- The propagation of EM waves through a photonic crystal depends on the wavelength; for certain wavelengths the propagation in the photonic crystal is forbidden (**Photonic Band Gap**)
- In case of very high structures (z-direction), the photonic crystal can be approximated as two-dimensional
- The **COMSOL Multiphysics RF Module** (2D, TE waves) is used to simulate light propagation through our photonic crystal structures



TM Bands of a rod-type Si photonic crystal:



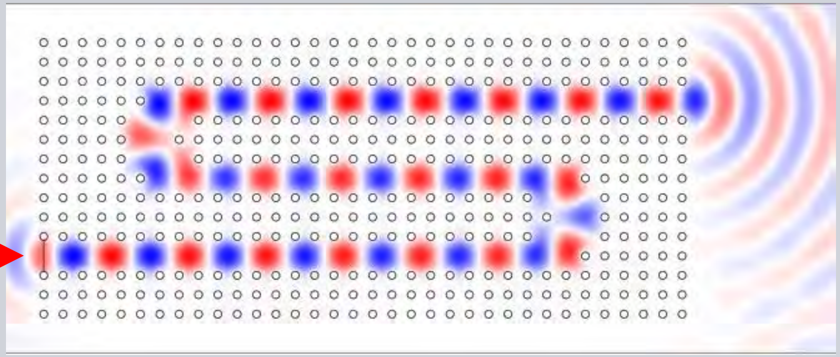


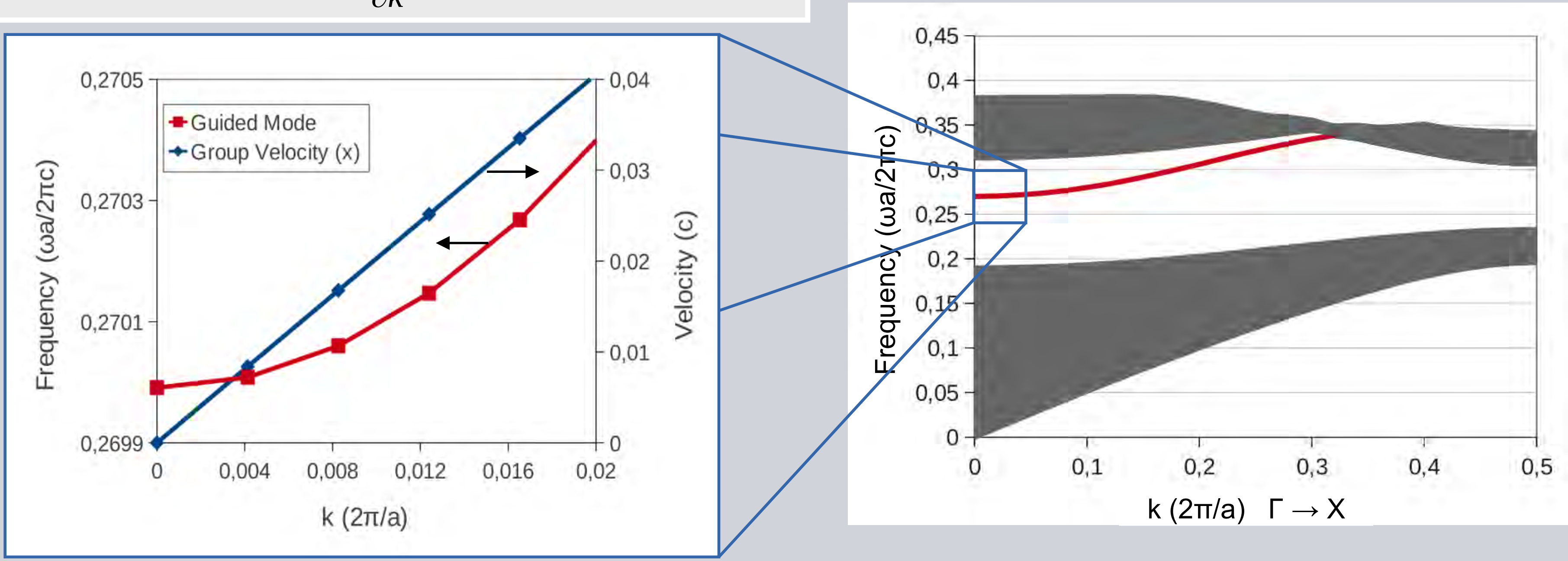
SIEMENS

Photonic crystal waveguides for gas detection

- A waveguide is created by removing a row of rods (line defect). It guides light, which's frequency lies in the bandgap of the photonic crystal
- The length of the waveguide can be increased by several bends:
  This increases the **absorption length**
- At certain frequencies the light propagates with an extremely slow group velocity (**slow light**):

$$v_G = \frac{\partial \omega}{\partial k}$$





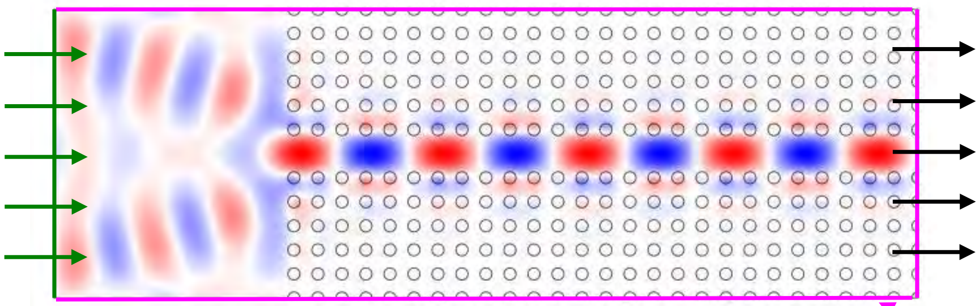
Simulation of light propagation through a photonic crystal waveguide

Calculation of the transmission spectrum:

1. Light propagation and coupling into a photonic crystal waveguide

Plane Wave
(Amplitude Ez = 1)
is applied to the
left boundary

Wavelength scan



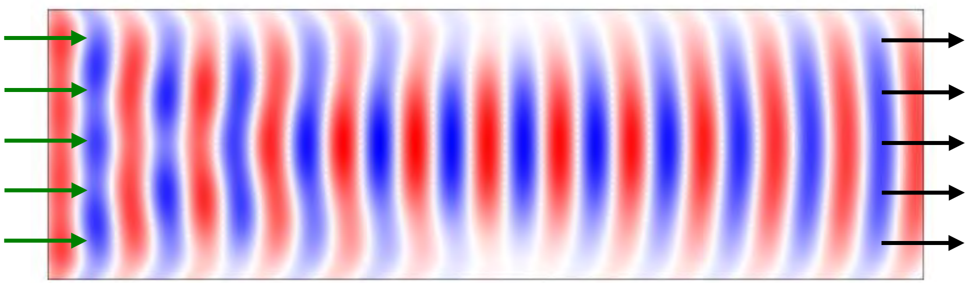
Power Outflow
(P_{out}) through the
right boundary is
calculated for each
wavelength

Scattering boundary condition

2. Light propagation in an empty air box of equal size

Plane Wave
is applied to the
left boundary

same wavelengths



Power Outflow
(P_{out}) is calculated

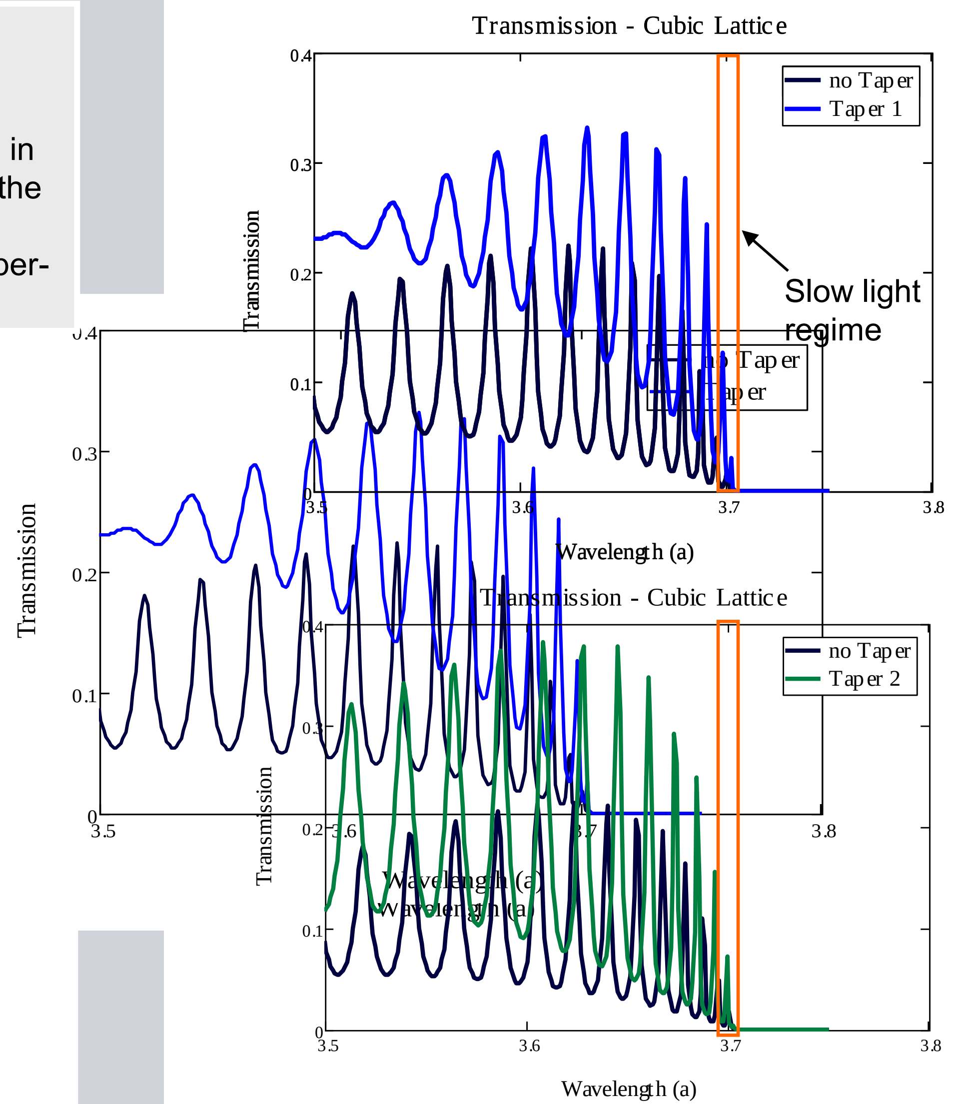
The Transmission through the waveguide is:

$$T = \frac{P_{out,WG}}{P_{out,Airbox}}$$

Coupling into photonic crystal waveguides

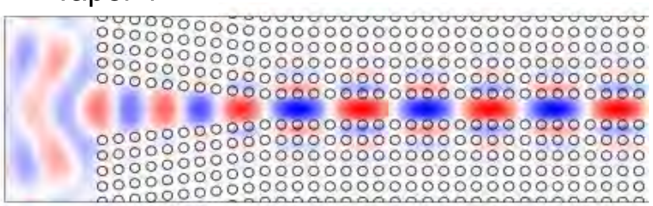
- Light is produced by an external light source
- → Coupling of light into the waveguide from “outside”

- Strong Fabry-Pérot Interferences can be observed in the transmission spectrum (wavelength in units of the lattice pitch a)
- The Transmission can be increased strongly by taper-like coupling geometries

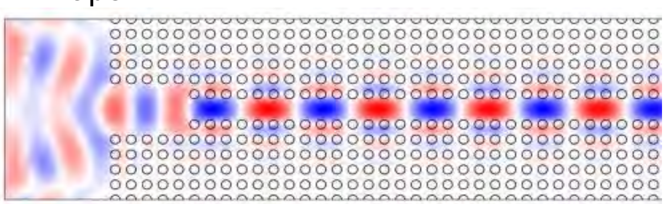


no Taper

Taper 1



Taper 2



Simulation of the gas detection with methane (700 ppm) at 7.625 µm

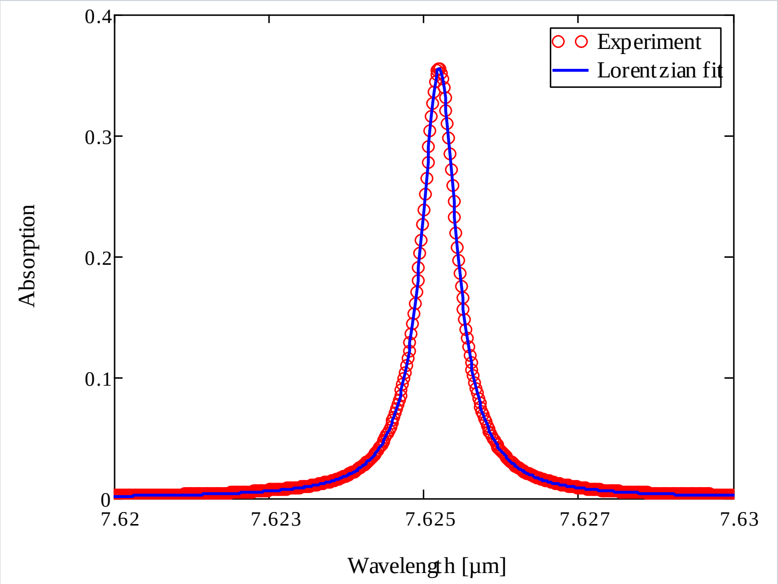
SIEMENS

To simulate the influence of a test gas (methane) on an optical gas sensor, two things are needed:

- Absorption cross section of methane at 7.625 µm, obtained from literature (HITRAN database):

$$\sigma_{Methane} = 4.375 \cdot 10^{-15} mm^2$$

- The shape of the absorption line at RT (obtained from a previous experiment with a conventional gas sensor)



The fit-function and the absorption cross section are used to calculate an expression for the light **extinction (κ)** as a function of the wavelength:

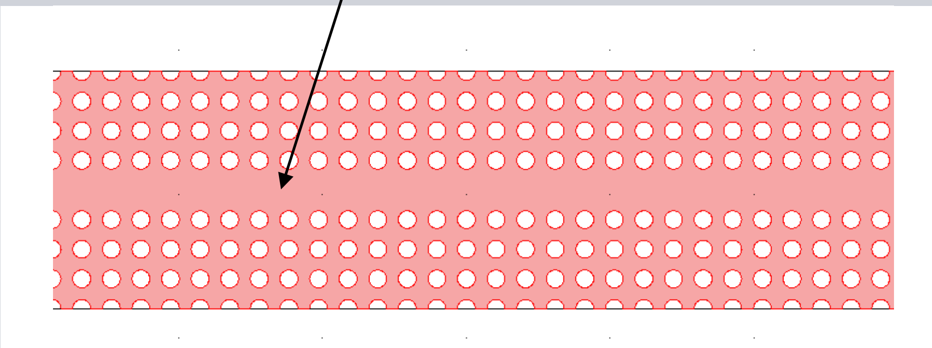
$$\kappa_{Methane}(\lambda) = \frac{7.625\mu m}{4 \cdot \pi^2 \cdot k_\alpha} \cdot \frac{b}{b^2 + (\lambda - 7.625\mu m)^2}$$

with: b = 3.5055 10^{-10}
k_α = 1.1056 10^{7}

Subsequently the complex refractive index n of air containing 700 ppm methane is:

$$n(\lambda) = 1 + i \cdot \kappa_{Methane}(\lambda)$$

This function is used in COMSOL to describe the material property of the **air-subdomain**:



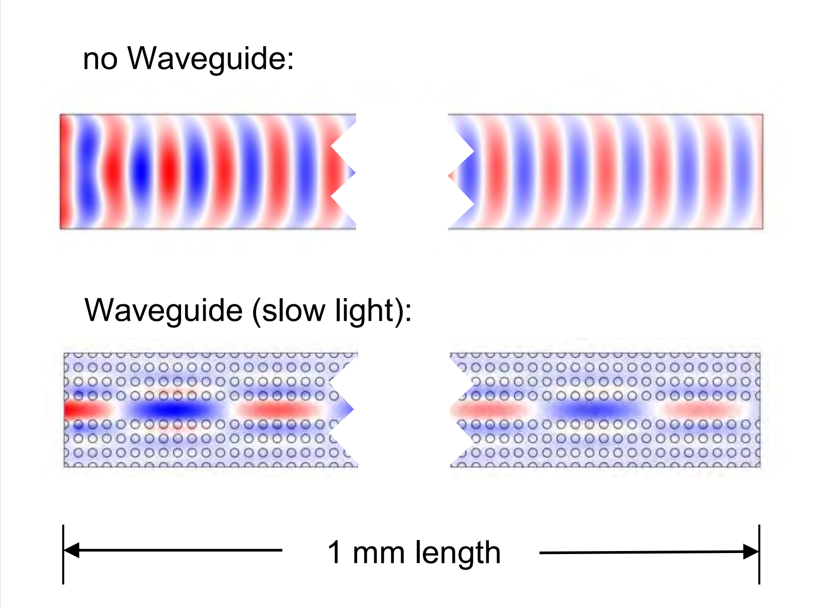
Simulation of the gas detection with methane (700 ppm) at 7.625 µm

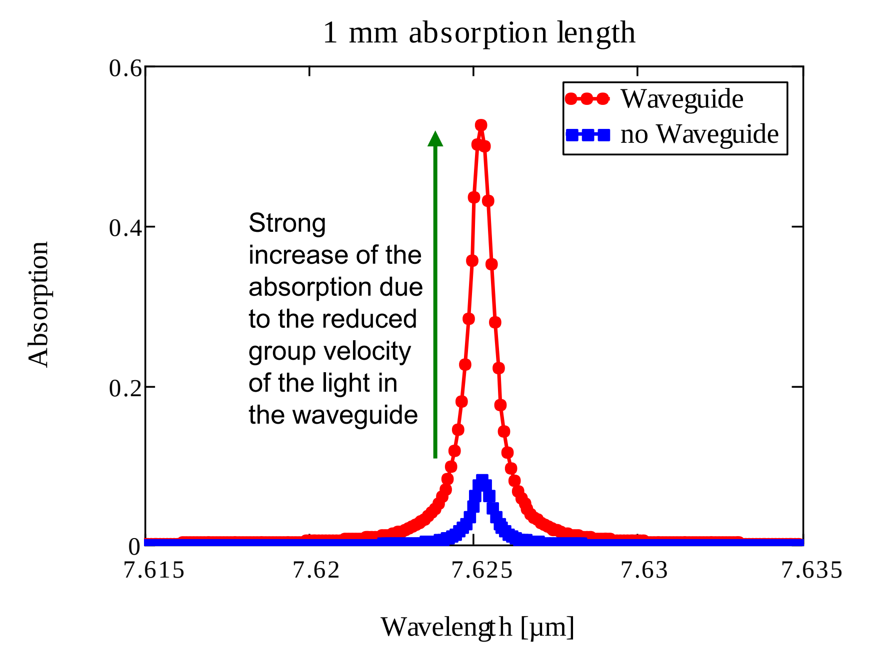
SIEMENS

The absorption due to methane is calculated by comparing the Power Outflow (P_{out}) of a structure containing methane to a structure containing only air (n = 1):

$$Absorption = 1 - \frac{P_{out,Methane}}{P_{out,Air}}$$

Comparing the absorption of a 1 mm long waveguide in slow light condition with an air box of the same length:





Conclusion

COMSOL Multiphysics (RF module) was successfully used to simulate:

- Light propagation though a bulk photonic crystal / photonic crystal waveguide
- Transmission spectra of photonic crystal waveguides to identify optimal coupling geometries
- Increased gas absorption in a photonic crystal waveguide due to slow light effects

Thank you for your attention !!!