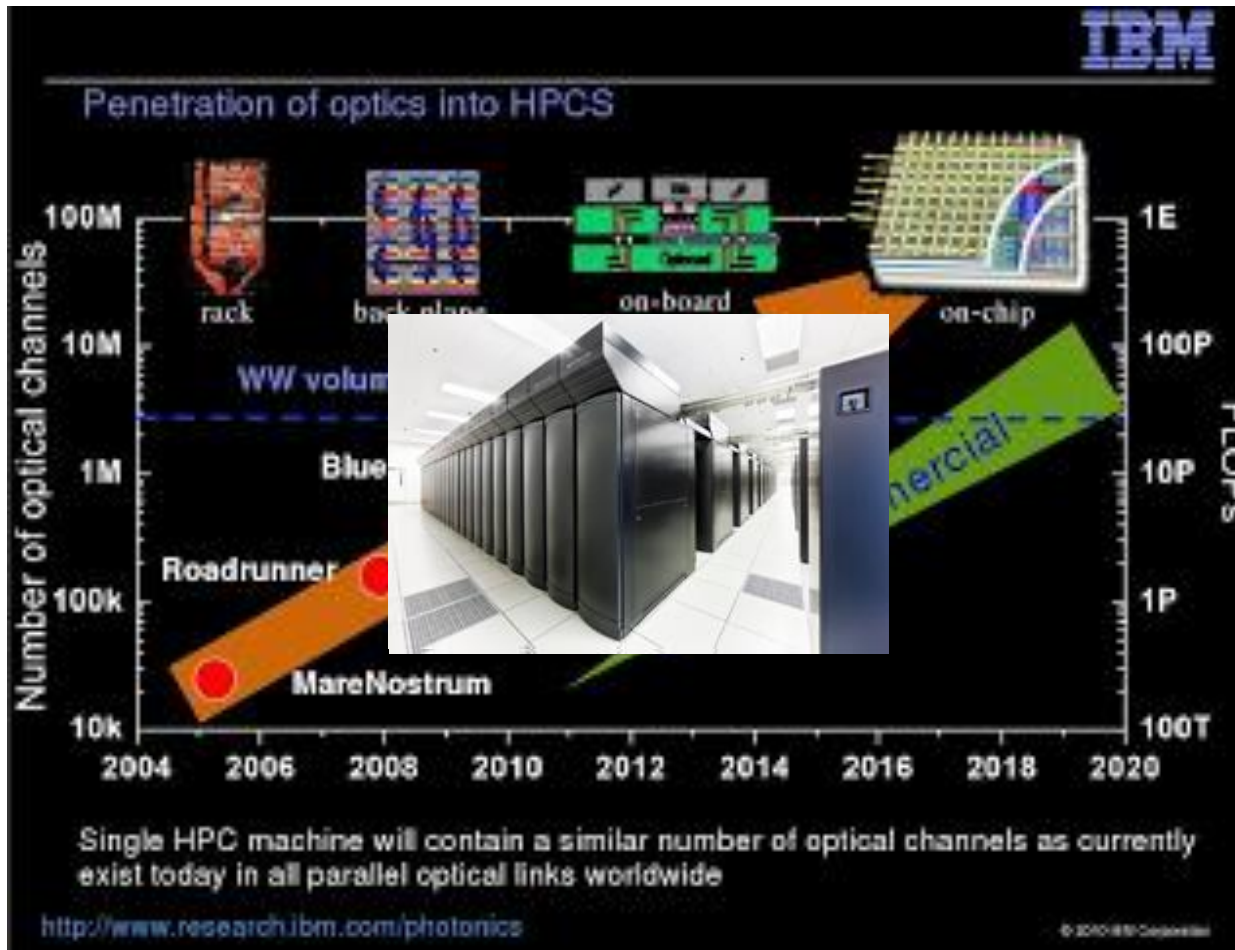


MODELOVÁNÍ PLANÁRNÍHO VLNOVODU S ABSORPČNÍ VRSTVOU

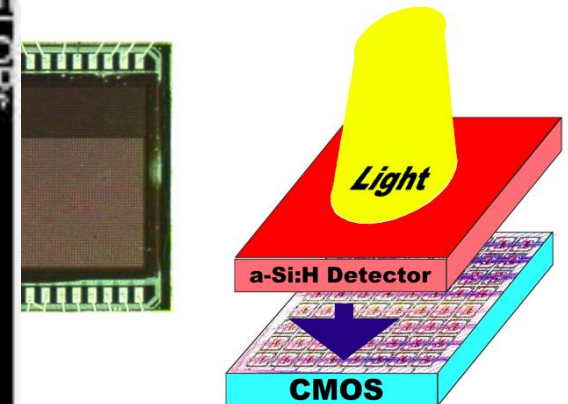
Vít Jirásek, Zdeněk Remeš, Václav Prajzler
Fyzikální ústav Akademie Věd České republiky

Hydrogenovaný amorfni křemík pro vlnovody



al.)
ated Circuits

ysrsch et al., Sensors, 2008

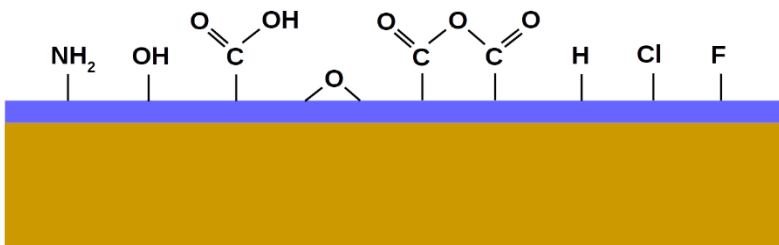


degradace v nepříznivých podmínkách – nutnost ochrany

Vrstvy nanokrystalického diamantu

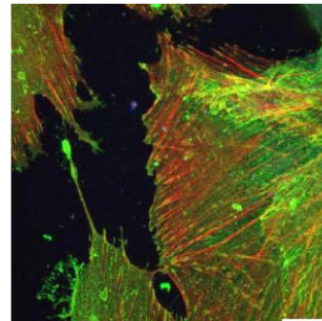
- MWCVD – chemická depozice z par podpořená MW plazma
- ochranná vrstva:
 - extrémně tvrdá
 - chemicky inertní
 - vysoce tepelně vodivá

□ NCD funkcionalizace

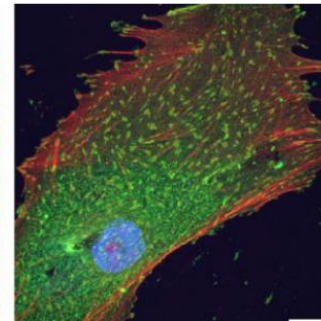


- smáčivost
- el. vodivost
- linkery

□ bio-compatibilita

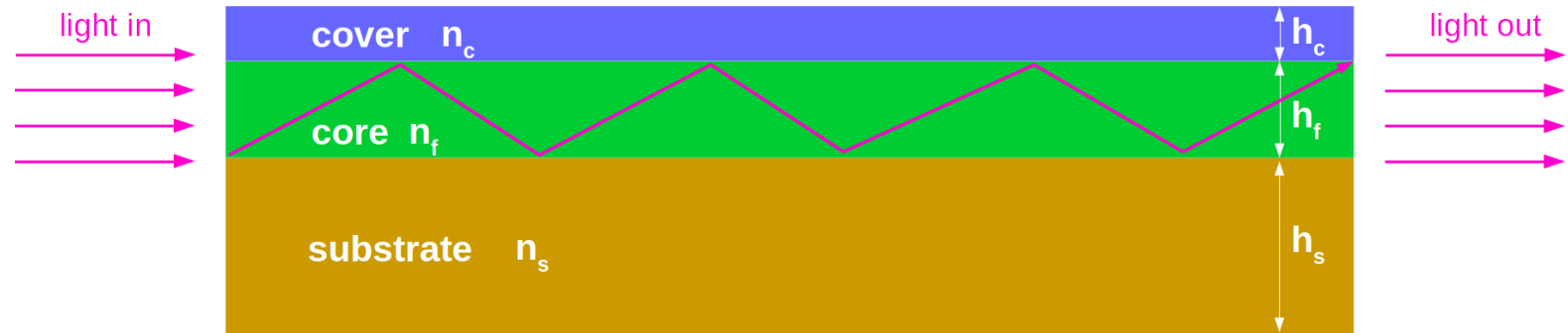


NCD H-term.



NCD O-term.

Planární optický vlnovod (POWVG)



podmínky šíření světla: $n_c < n_f > n_s$

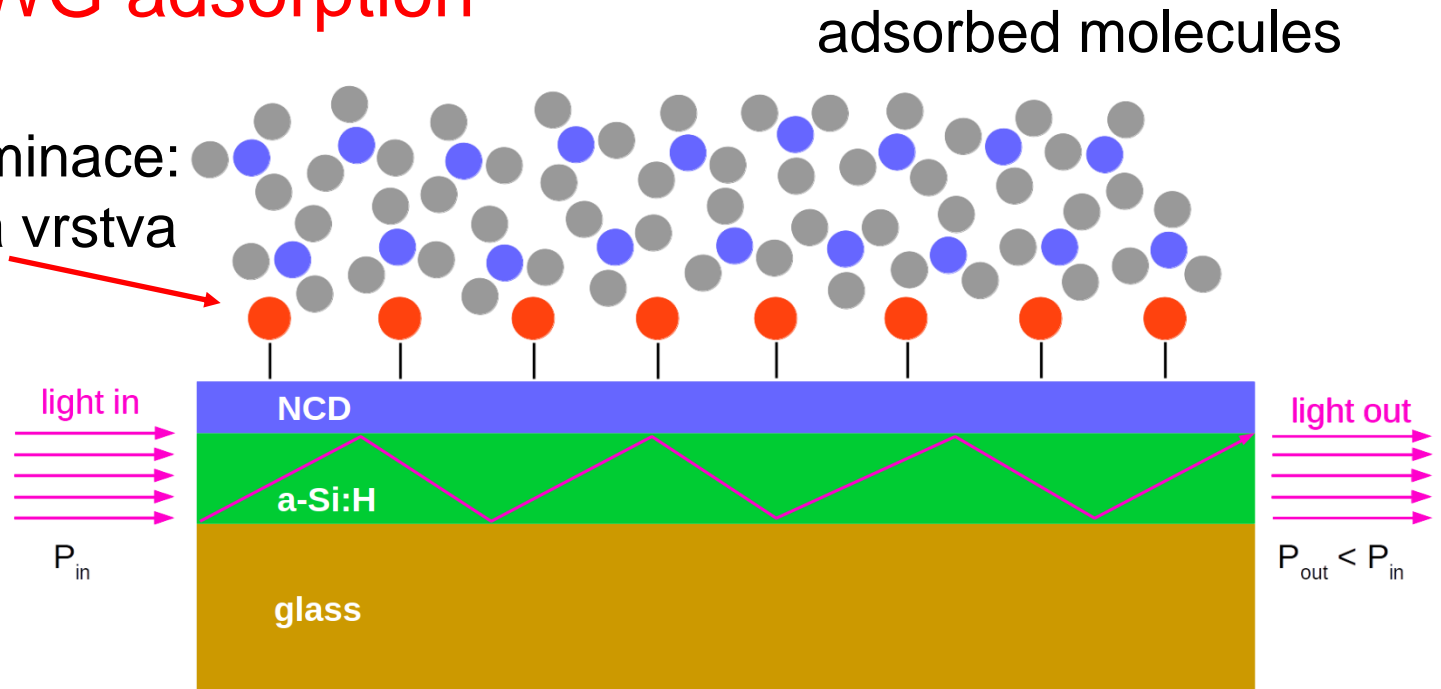
+ příčná rezonance

- mode: a stable field distribution in the propagation direction with only a periodic transverse dependence
 - TE a TM módy = s- nebo p-polarizace
- jednomódový vlnovod (single-mode): λ, h_f, n_i

POWG pokryté NCD diamantem

NCD-POWG adsorption monitor

povrchová terminace:
funkční citlivá vrstva



- absorpční vrstva (několik nm): páry & kapaliny
- zeslabení optického signálu
- integrace & citlivost

Řešení modifikované disperzní rovnice

- model planárního vlnovodu: výška \ll šířka \longrightarrow 2D
- efektivní index lomu

$$\frac{2\pi h_f}{\lambda_0} \sqrt{n_f^2 - n_{eff}^2} = \arctan\left(p_{fs} \sqrt{\frac{n_{eff}^2 - n_s^2}{n_f^2 - n_{eff}^2}}\right) + \arctan\left(p_{fc} \sqrt{\frac{n_{eff}^2 - n_c^2}{n_f^2 - n_{eff}^2}}\right) + m\pi$$

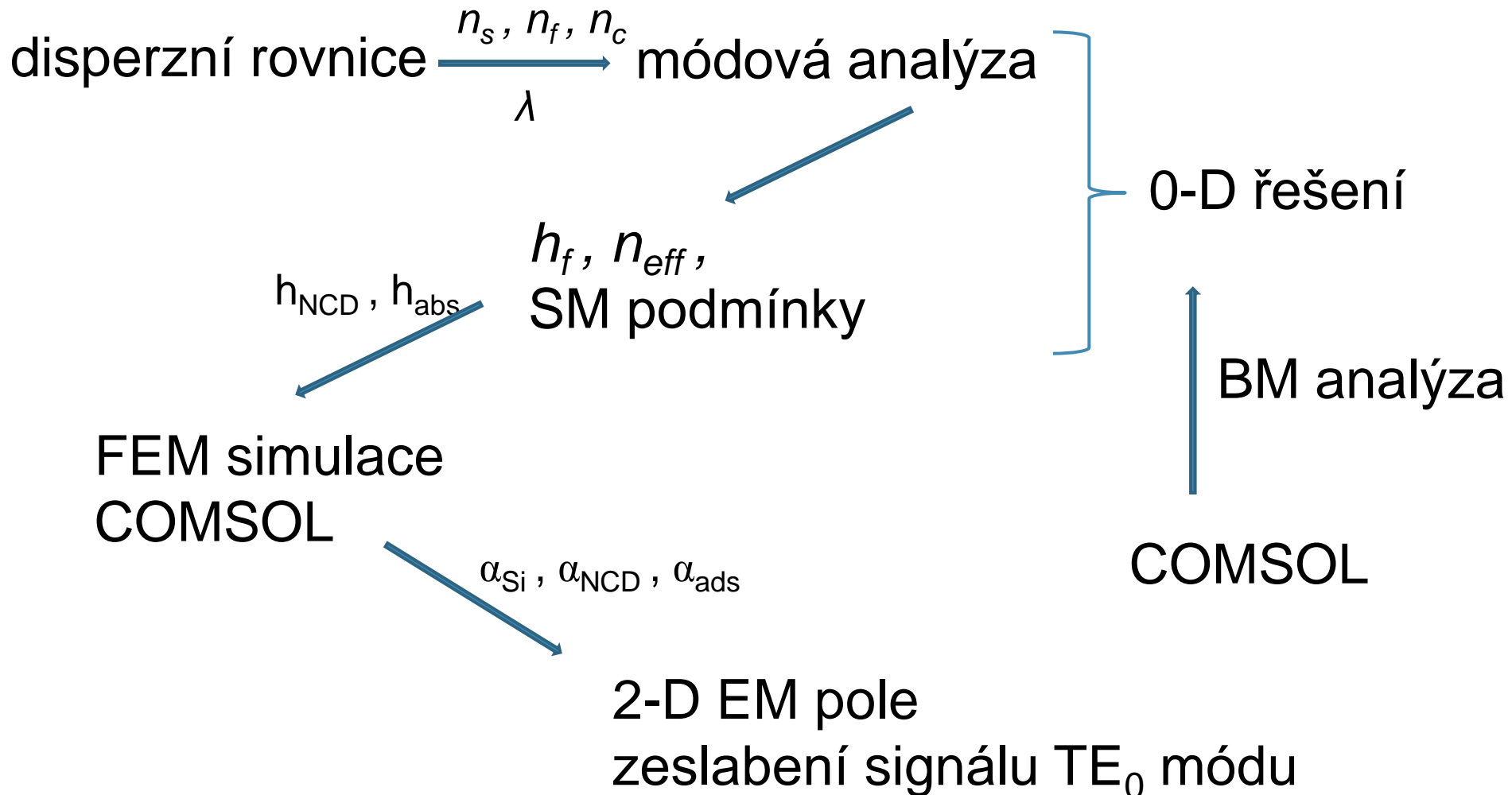
$m = 0, 1, 2, \dots$

TE: $p_{fs} = p_{fc} = 1,$

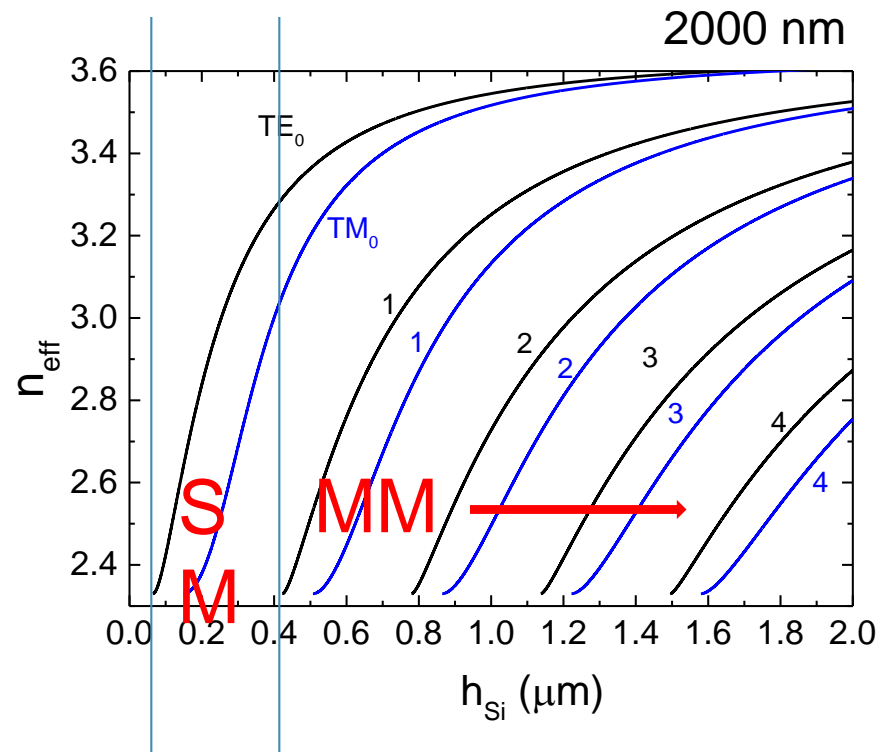
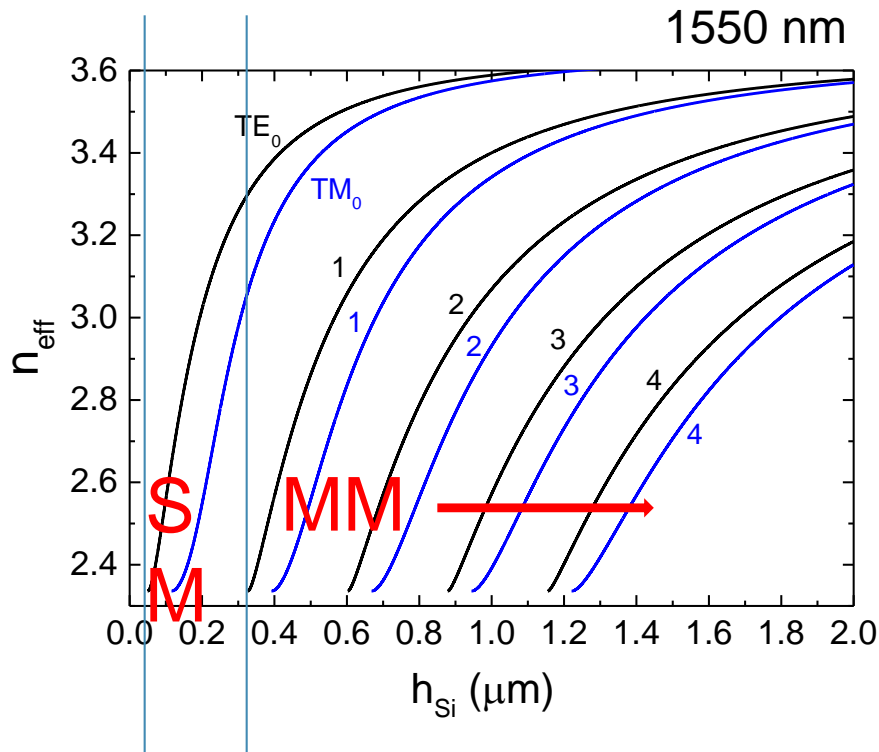
TM: $p_{fs} = \frac{n_f^2}{n_s^2}, \quad p_{fc} = \frac{n_f^2}{n_c^2},$

- bez optické absorpce

POWG design & simulace



Výpočty módů



- 1-módový vlnovod pro 1550-2000 nm:

$$h_{\text{Si}} = 150\text{-}320 \text{ nm}$$

- 280 nm zvoleno pro FEM simulace

FEM simulace

- COMSOL Multiphysics (RF module, verze

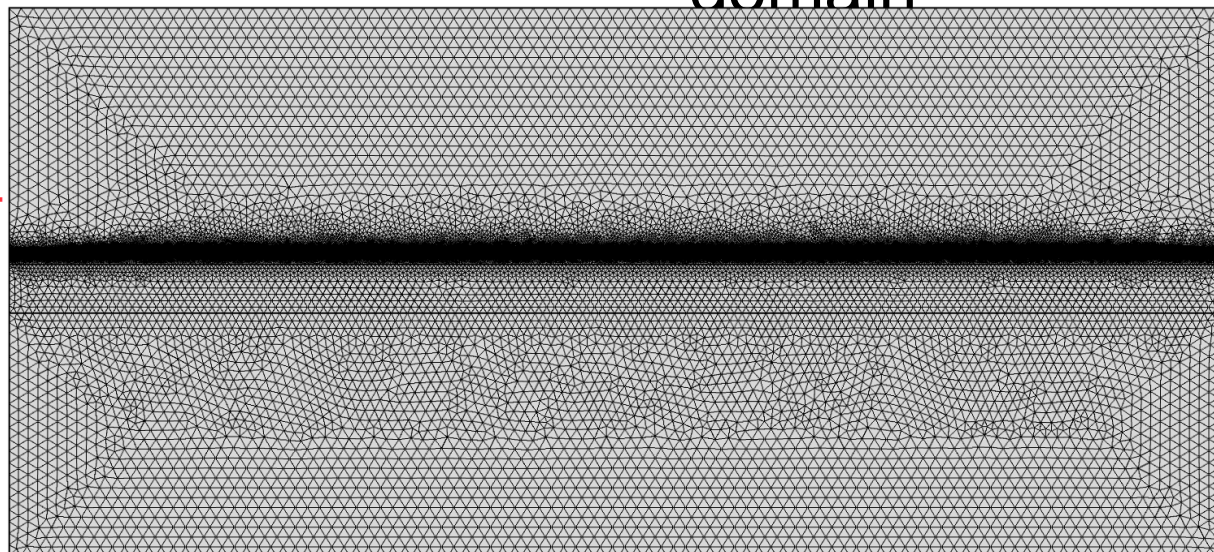
$$\nabla \times (\nabla \times \tilde{\mathbf{E}}) - k_0 \epsilon_r \tilde{\mathbf{E}} = 0$$

$$\tilde{\mathbf{E}}(x, y, z) = \tilde{\mathbf{E}}(x, y) \exp(-ik_z z)$$

- nemagnetické prostředí

- řešení ve frequency domain

absorber



0-50 nm

200-300 000 FEM elementů

Define, geometry, parameter

The screenshot displays the COMSOL Multiphysics software interface. The title bar reads "D-a_SI_abs.mph - COMSOL Multiphysics". The menu bar includes "File", "Edit", "Windows", "Options", "Tools", and "Help". The toolbar shows various icons for file operations and model building. The "Component 1" dropdown is set to "Electromagnetic Waves, Frequency Domain".

The "Model Builder" tree on the left shows the following structure:

- D-a_SI_abs.mph (root)
 - Global Definitions
 - Parameters
 - Materials
 - Component 1 (comp1)
 - Definitions
 - Geometry 1
 - Materials
 - Electromagnetic Waves, Frequency Domain (ewfd)
 - Mesh 1
 - Study 1
 - Step 1: Boundary Mode Analysis
 - Step 2: Boundary Mode Analysis 1
 - Step 3: Frequency Domain
 - Solver Configurations
 - Results
 - Data Sets
 - Derived Values
 - Tables

The "Parameters" table in the "Settings" pane is as follows:

Name	Expression	Value	Description
lambda0	1550[nm]	1.55E-6 m	Wavelength
n_d	2.336	2.336	Refractive index, core
k_d	7.5e-4	7.5E-4	
n_si	3.65	3.65	
k_si	2.14e-6	2.14E-6	
n_sklo	1.5	1.5	Refractive index, clad
h_d	0.050[um]	5E-8 m	
h_sklo	1[um]	1E-6 m	Thickness, film
h_si	0.280[um]	2.8E-7 m	Thickness, cladding
h_air	1[um]	1E-6 m	
w_slab	5[um]	5E-6 m	Slab width
f0	c_const/lambda0	1.9341E14 1/s	Frequency
h_abs	0.005	0.005	
n_abs	2.336	2.336	

Navigation icons (up, down, search, save) are visible below the table. The "Name:" field is empty.

Definice, geometrie, parametry

The screenshot displays the COMSOL Multiphysics software interface. The title bar reads "D-a_Si_abs.mph - COMSOL Multiphysics". The menu bar includes "File", "Edit", "Windows", "Options", "Tools", and "Help". The toolbar contains various icons for file operations and simulation controls. The main window is divided into several panes:

- Model Builder:** Shows a hierarchical tree of the model. The "Electromagnetic Waves, Frequency Domain (ewfd)" node is selected and highlighted in orange. Underneath it, several physics nodes are listed: "Wave Equation, Electric 1", "Perfect Electric Conductor 1", "Initial Values 1", "Port 1", and "Port 2". A "Mesh 1" node is also visible under "Component 1 (comp1)".
- Settings/Properties:** This pane is active and shows the configuration for the "Electromagnetic Waves, Frequency Domain" study. The "Label" is "Electromagnetic Waves, Frequency Domain" and the "Name" is "ewfd". Under the "Domain Selection" section, the "Selection" is set to "All domains". A table lists domains 1 through 5, with a power button icon next to domain 1, indicating it is active. The "Equation" section shows the "Equation form" set to "Study controlled" and "Show equation assuming" set to "Study 1, Boundary Mode Analysis".

At the bottom of the Settings pane, the following equations are displayed:

$$\nabla \times \mu_r^i (\nabla \times \mathbf{E}) - k_0^2 (\epsilon_r - \frac{j\sigma}{\omega\epsilon_0}) \mathbf{E} = 0$$
$$\lambda = -j\beta - \delta_z$$
$$\mathbf{E}(x,y,z) = \tilde{\mathbf{E}}(x,y)e^{-ik_z z}$$

Okrajové podmínky

The screenshot displays the COMSOL Multiphysics software interface for a model named "D-a_Si_abs.mph". The main window is titled "Electromagnetic Waves, Frequency Domain". The left sidebar shows the Model Builder tree with the following structure:

- D-a_Si_abs.mph (root)
 - Global Definitions
 - Parameters
 - Materials
 - Component 1 (comp1)
 - Definitions
 - Geometry 1
 - Materials
 - Electromagnetic Waves, Frequency Domain (ewfd)
 - Wave Equation, Electric 1
 - Perfect Electric Conductor 1
 - Initial Values 1
 - Port 1**
 - Port 2
 - Mesh 1
 - Study 1
 - Step 1: Boundary Mode Analysis
 - Step 2: Boundary Mode Analysis 1
 - Step 3: Frequency Domain
 - Solver Configurations
 - Solution 1
 - Compile Equations: Boundary Mode Analysis
 - Dependent Variables 1
 - Eigenvalue Solver 1
 - Solution Store 1
 - Compile Equations: Boundary Mode Analysis 1
 - Dependent Variables 2
 - Eigenvalue Solver 2
 - Solution Store 2
 - Compile Equations: Frequency Domain
 - Dependent Variables 3
 - Stationary Solver 1
 - Direct

The right sidebar shows the Properties panel for the selected "Port 1" entity. The "Boundary Selection" section is set to "Manual" and lists active boundaries 1, 3, 5, 7, and 9. The "Equation" section shows the wave equation: $n \times \nabla \times E - j\beta n \times E \times n = 0$. The "Port Properties" section includes:

- Port name: 1
- Type of port: Numeric
- Wave excitation at this port: On
- Specify deposited power:
- Port input power: P_{in} 1 W
- Port phase: θ_{in} 0 rad

On the far right, a plot shows a vertical gray bar with a blue line at the top, representing the port excitation profile. The y-axis ranges from -0.5 to 3.5.

Model Builder

- ← → 🔍 ⌵ ⌶ ⌷
- ▼ D-a_Si_abs.mph (root)
 - ▼ Global Definitions
 - P_i Parameters
 - Materials
 - ▼ Component 1 (comp1)
 - ▶ Definitions
 - ▶ Geometry 1
 - ▶ Materials
 - ▶ Electromagnetic Waves, Frequency Domain (ewfd)
 - ▼ Mesh 1
 - Size
 - ▶ Study 1
 - ▶ Results

Settings Properties

Size

Build Selected Build All

Label: Size

Element Size

Calibrate for:
General physics

Predefined Normal

Custom

Element Size Parameters

Maximum element size: μm

Minimum element size: μm

Maximum element growth rate:

Curvature factor:

Resolution of narrow regions:

Dejství řešení šíření světla (Frequency

D-a_SI_abs.mph - COMSOL Multiphysics

File Edit Windows Options Tools Help

Component 1 Π a= f(x) Electromagnetics

Definitions Geometry Materials Physics Mesh Study Results

Model Builder

- D-a_SI_abs.mph (root)
 - Global Definitions
 - Π Parameters
 - Materials
 - Component 1 (comp1)
 - Study 1
 - Step 1: Boundary Mode Analysis**
 - Step 2: Boundary Mode Analysis 1
 - Step 3: Frequency Domain
 - Solver Configurations
 - Results
 - Data Sets
 - Derived Values
 - Tables
 - Electric Field (ewfd)
 - 1D Plot Group 2
 - Export
 - Reports

Settings Properties

Boundary Mode Analysis

Compute Update Solution

Label: Boundary Mode Analysis

Study Settings

Transform: Effective mode index

Port name: 1

Mode analysis frequency: f0

Mode search method: Region

Approximate number of modes: 4

Maximum number of modes: 4

Perform consistency check

Search region

Smallest real part: n_d

Largest real part: n_Si

Smallest imaginary part: 0

Largest imaginary part: 0

Postprocessing

Plot (F8)

Label:

Data

Data set:

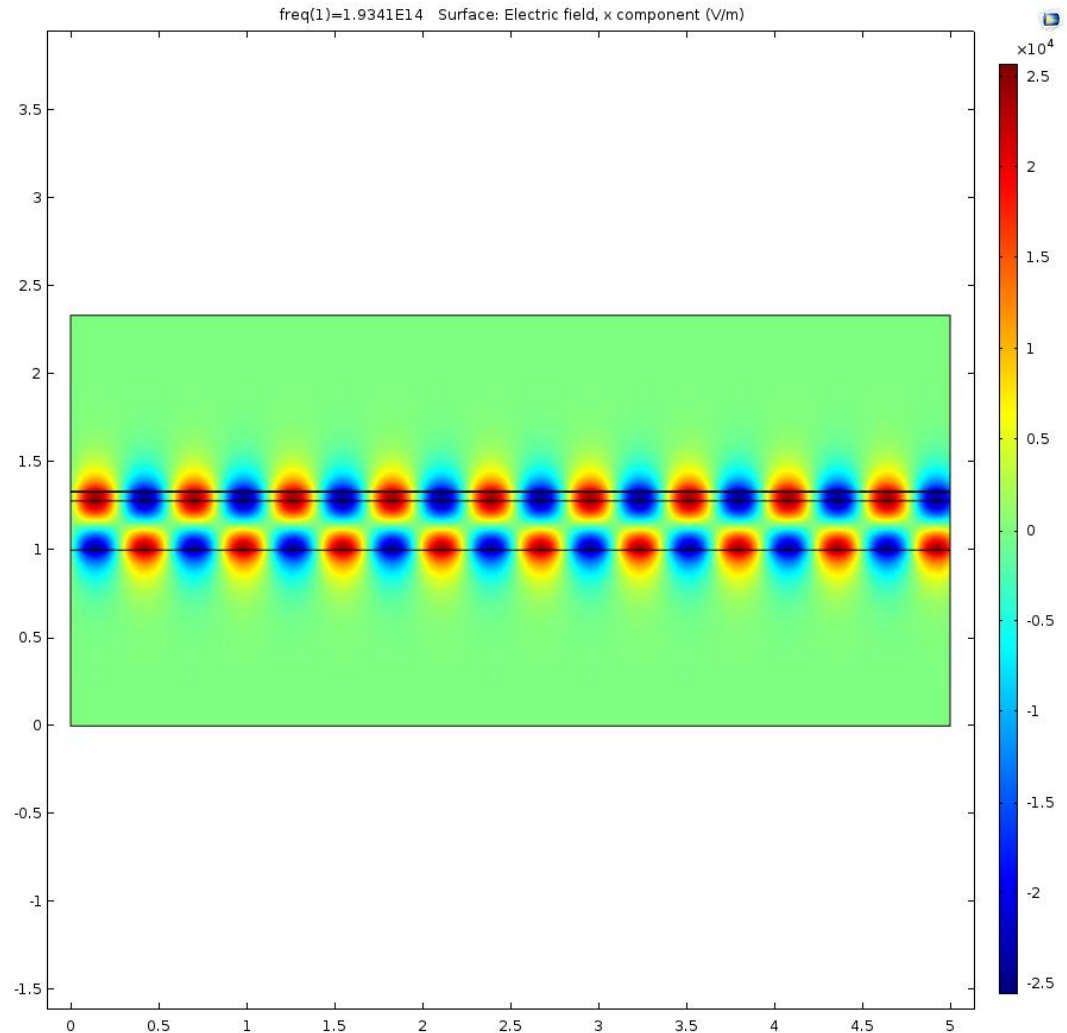
Parameter value (freq (Hz)):

Expression

Expression:

Unit:

Description:



Postprocessing

Plot (F8)

Label: Surface 1

Data

Data set: Study 1/Solution 1

Parameter value (freq (Hz)): 1.9341E14

Expression

Expression:

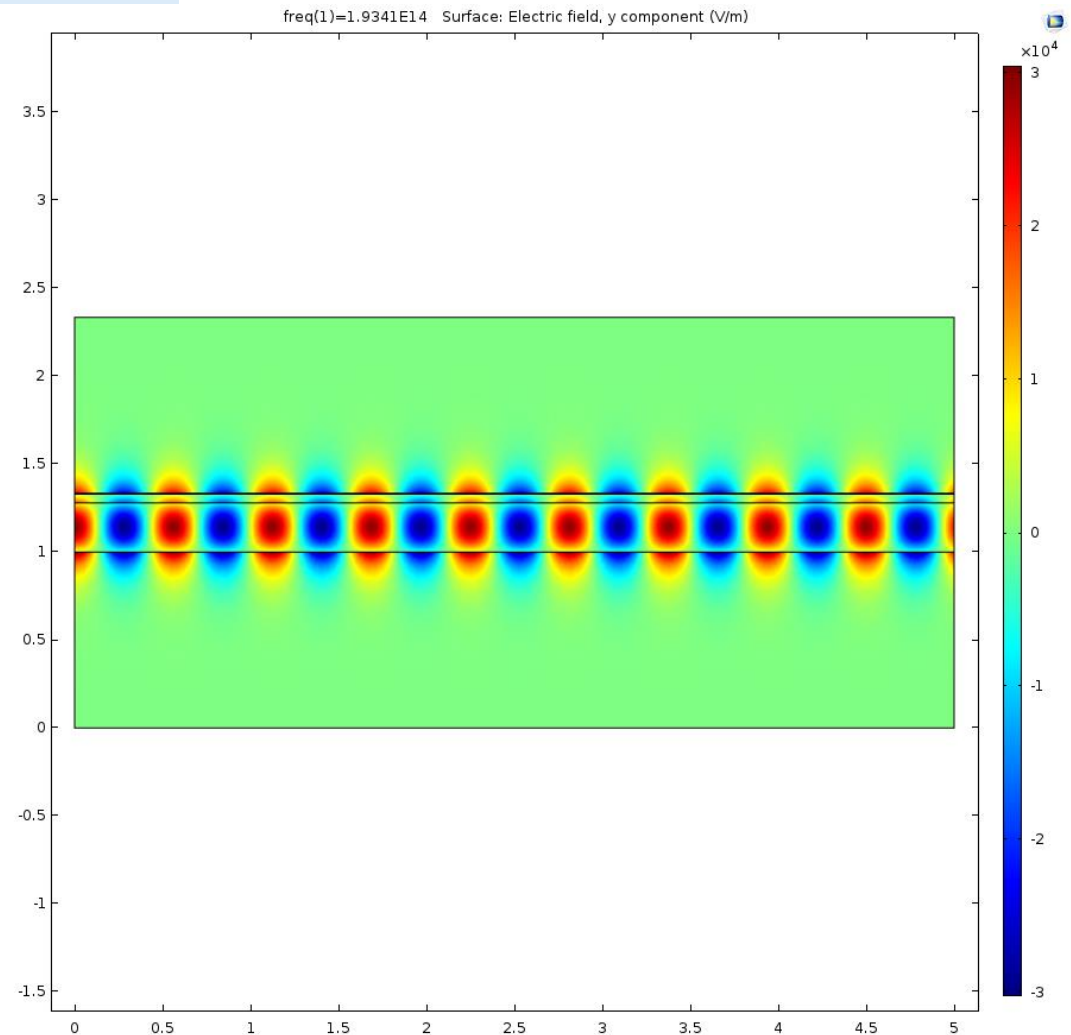
ewfd.Ey

Unit:

V/m

Description:

Electric field, y component



Postprocessing

Plot (F8)

Label: Surface 1

▼ Data

Data set: Study 1/Solution 1

Parameter value (freq (Hz)): 1.9341E14

▼ Expression

Expression:

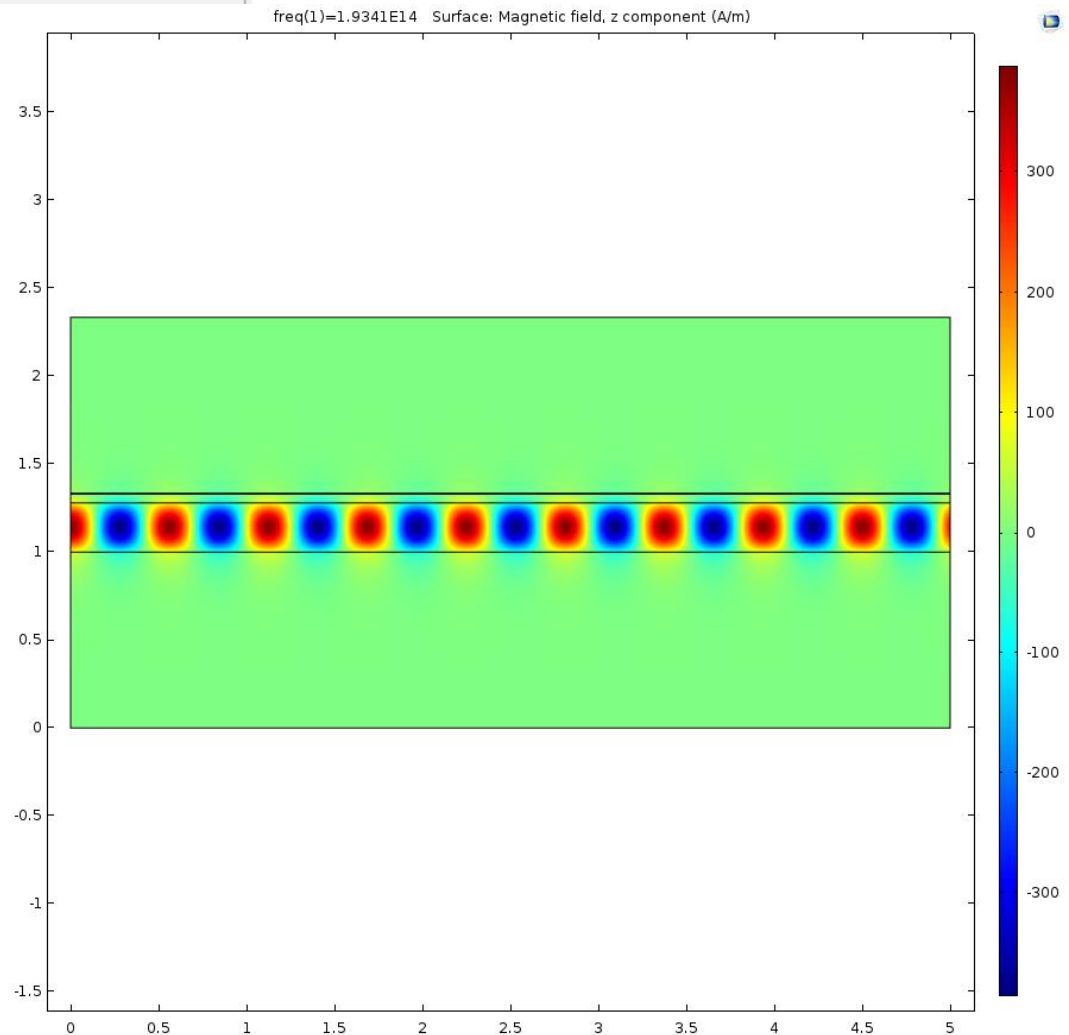
ewfd.Hz

Unit:

A/m

Description:

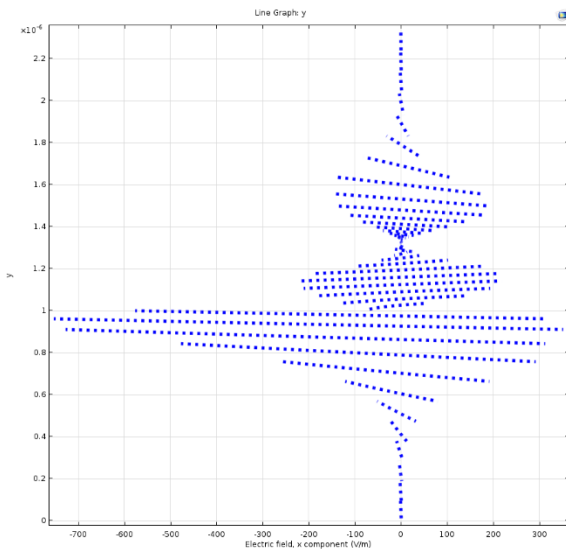
Magnetic field, z component



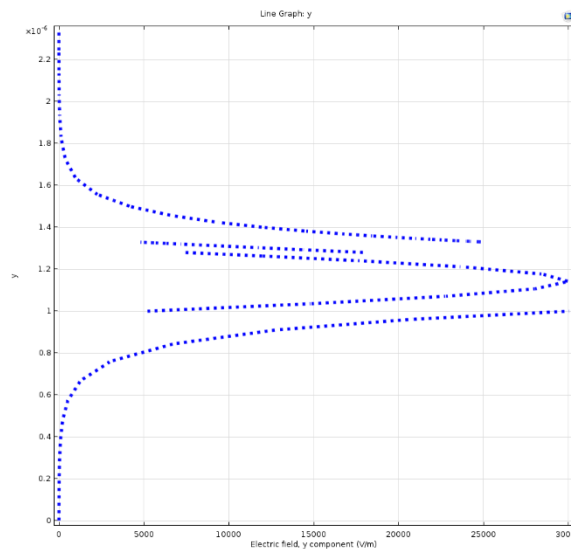
Postprocessing – profil módu

- mód TE_0
- $n_{\text{eff}} = 3.026$
- podél Portu 1
- dostupné až po vyřešení celé struktury

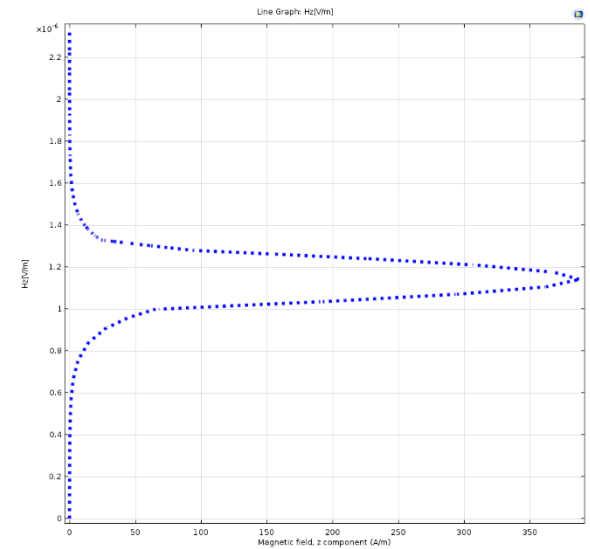
E_x



E_y



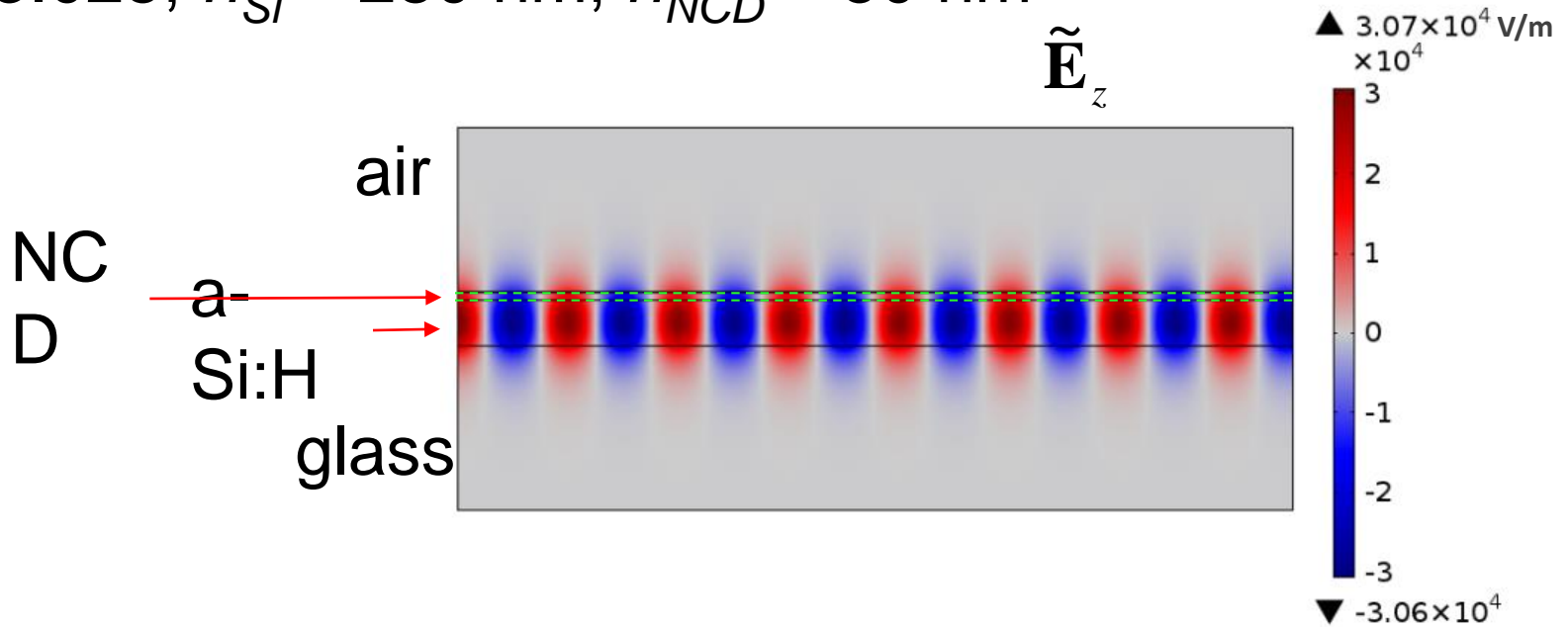
H_z



Výsledky simulace POWG

šíření světla v TE_0 módu při 2000 nm

$$n_{eff} = 3.025, h_{Si} = 280 \text{ nm}, h_{NCD} = 50 \text{ nm}$$



- evanescentní vlna vyhasínající ve vzduchu a ve skle
- monitorování nm-vrstvy bude možné

Výsledky simulací – útlum světla

útlum signálu: $att[dB/cm] = -\frac{10}{L} \log \frac{P_{out}}{P_{in}}$ L - délka
vlnovodu ve
směru šíření

COMSOL: S_{xy} parametry $S_{21} = \frac{\sqrt{P_{out}}}{\sqrt{P_{in}}}$ $S_{21}dB = 20 \log S_{21}$
(ewfd.S21) (ewfd.S21dB)

relativní pokles výkonu: $\frac{P_{out}}{P_{in}} = S_{21}^2$

útlum signálu: $att = -\frac{S_{21}dB}{L}$

absorpce: obecně komplexní S-parametry $\bar{S} = \sqrt{S_{Re}^2 + S_{Im}^2}$

S – parametry – zeslabení

The screenshot displays the COMSOL Multiphysics software interface. On the left is the 'Model Builder' tree, showing a project named 'D-a_Si_abs.mph (root)'. Under 'Component 1 (comp1)', the 'Electromagnetic Waves, Frequency Domain (ewfd)' interface is selected. The 'Results' section is expanded to show 'Derived Values' > 'Line Average 1'. The 'Evaluate' dialog box is open, showing the following configuration:

- Label:** Line Average 1
- Data:** Data set: Study 1/Solution 1; Parameter selection (freq): From list; Parameter values (freq (Hz)): 1.9341E14
- Selection:** Selection: Manual; Active: 12, 13, 14, 15, 16
- Expression:** Expression: ewfd.S21dB; Unit: dB

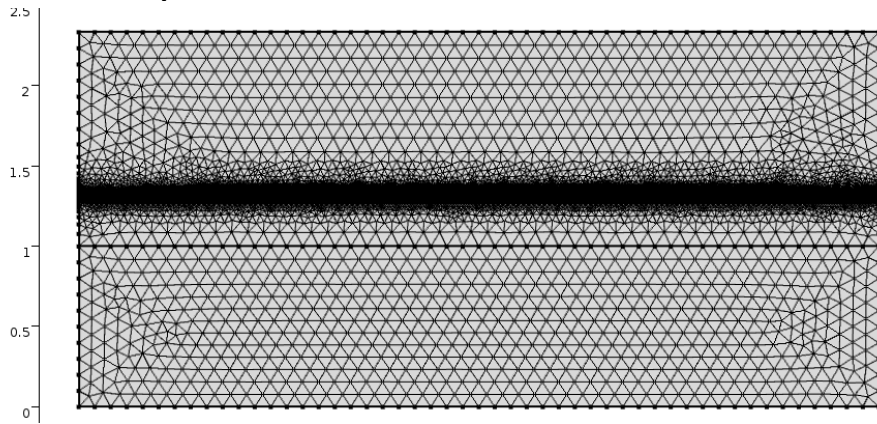
On the right, a table displays the results of the evaluation:

freq (Hz)	S-parameter, 21 component (dB)	S-parameter, dB
1.9341E14	0.75200+0.65653i	-0.015054

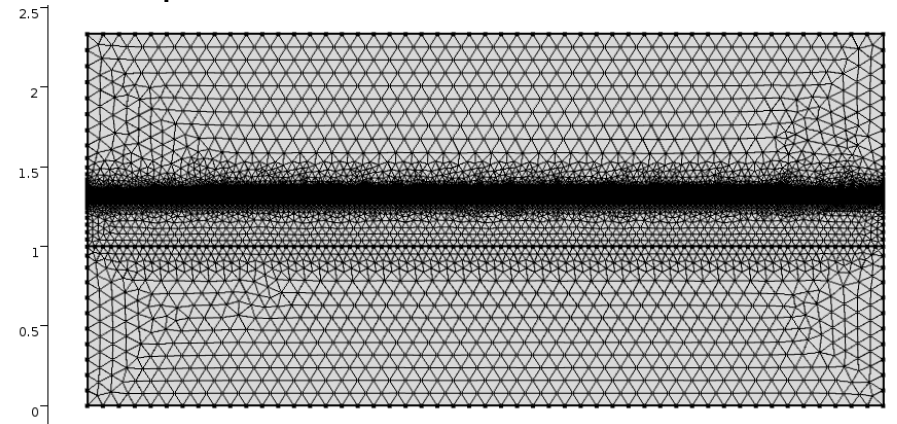
Vliv kvality sítě

maximální velikost prvku: λ/n_i

$n_i = 10$



$n_i = 40$



n_i ($\lambda = 1550$)	prvků	neff	S21dB bez absorpční vrstvy(dB)
10	198314	3.207	-0.004861
20	198572	3.207	-0.004852
40	200520	3.207	-0.004846
60	203936	3.207	-0.004845

Vliv kvality sítě

rozměr prvku v absorpční vrstvě: $h_{\text{abs}}/n_{\text{dabs}}$

$\lambda = 2000 \text{ nm}$, $h_{\text{abs}} = 5 \text{ nm}$, absolutní max. rozměr prvku = $\lambda/20$

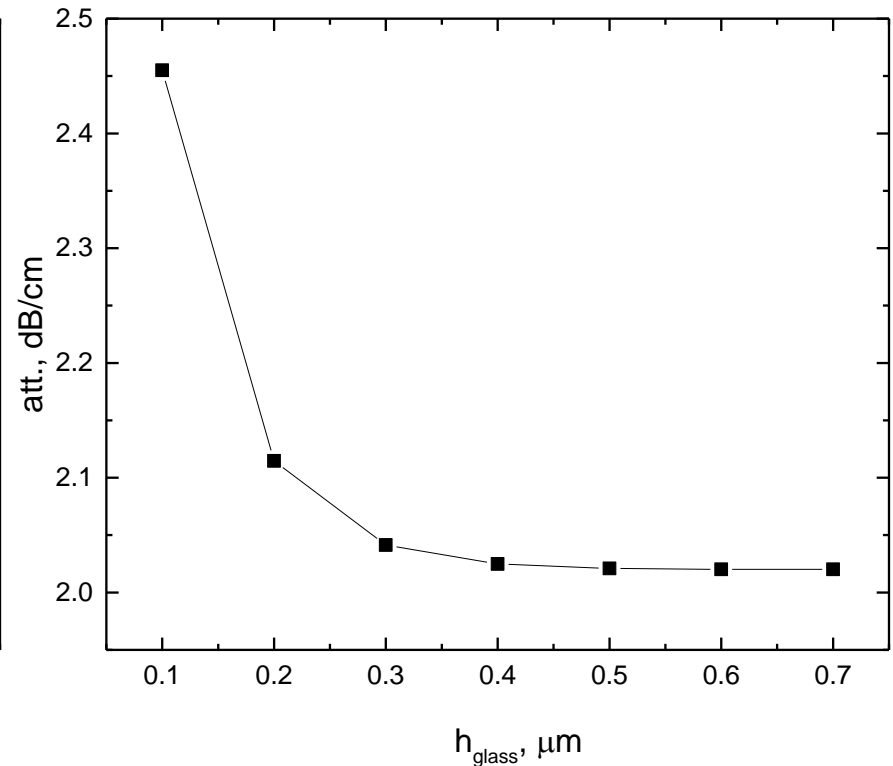
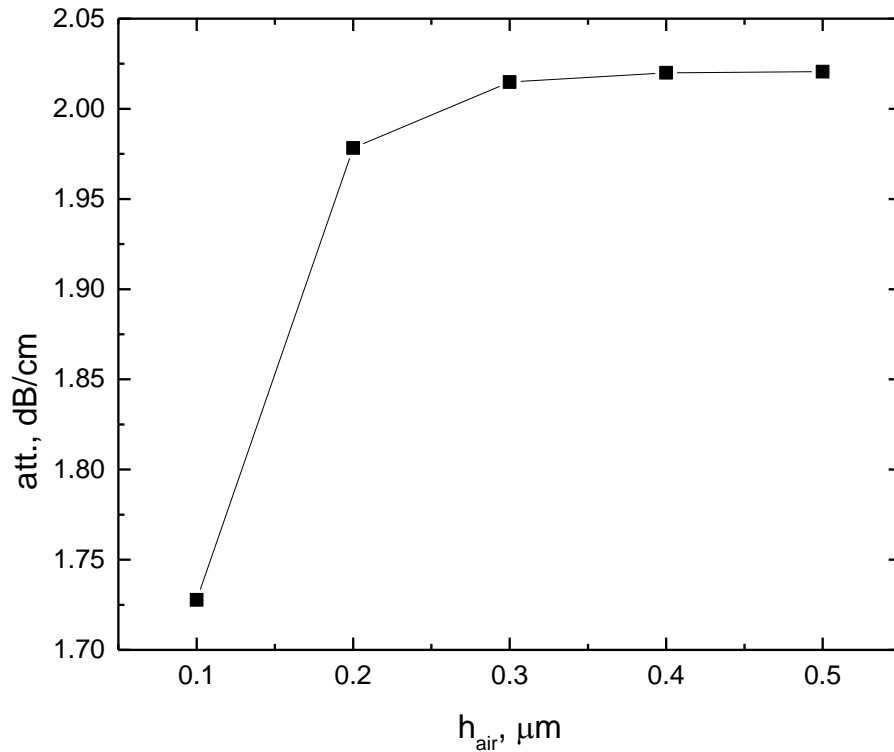
n_{dabs}	prvků	abs koef., cm^{-1}	S21dB (dB)	útlum (dB/cm)
7	322226	62.8	-0.0010103	2.0206
5	198314	62.8	-0.0010103	2.0206
3	105968	62.8	-0.0010103	2.0206
2	65460	62.8	-0.0010103	2.0206
1	29620	62.8	-0.0010104	2.0208
3	105968	0	-0.0007812	1.5625

Vliv vzduchu a skla

výška přidané vzduchové vrstvy:
výška spodního skla:

h_{air}

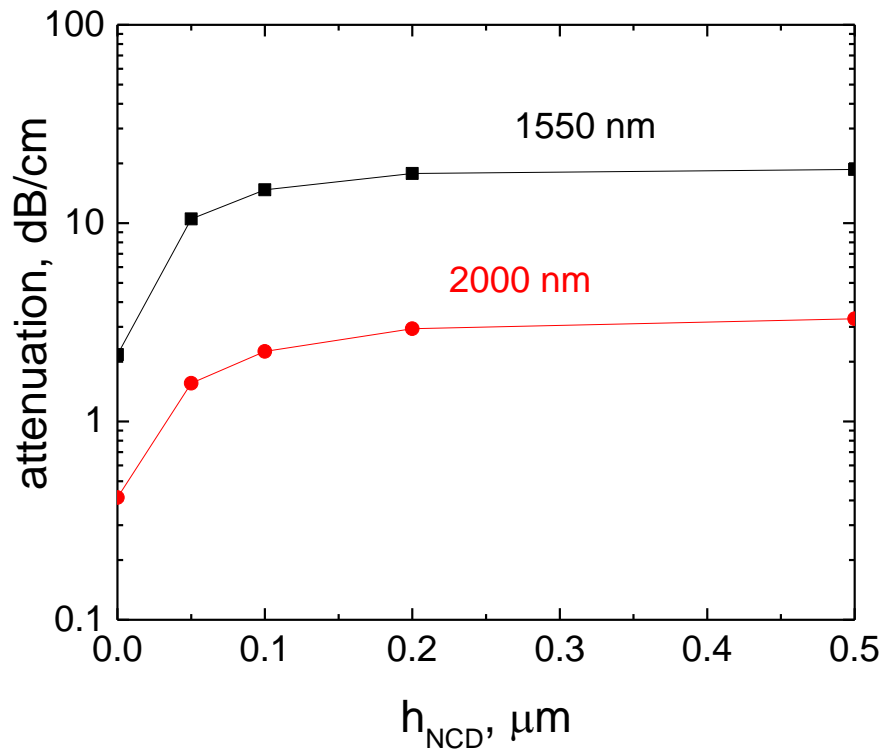
h_{glass}



Výsledky simulací– útlum v NCD

bez absorpční vrstvy

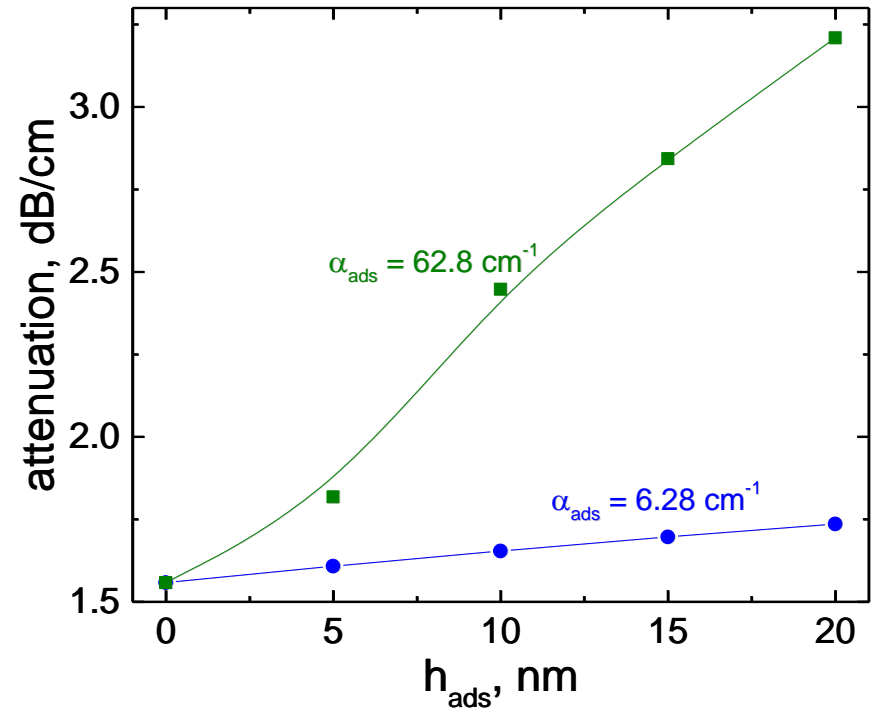
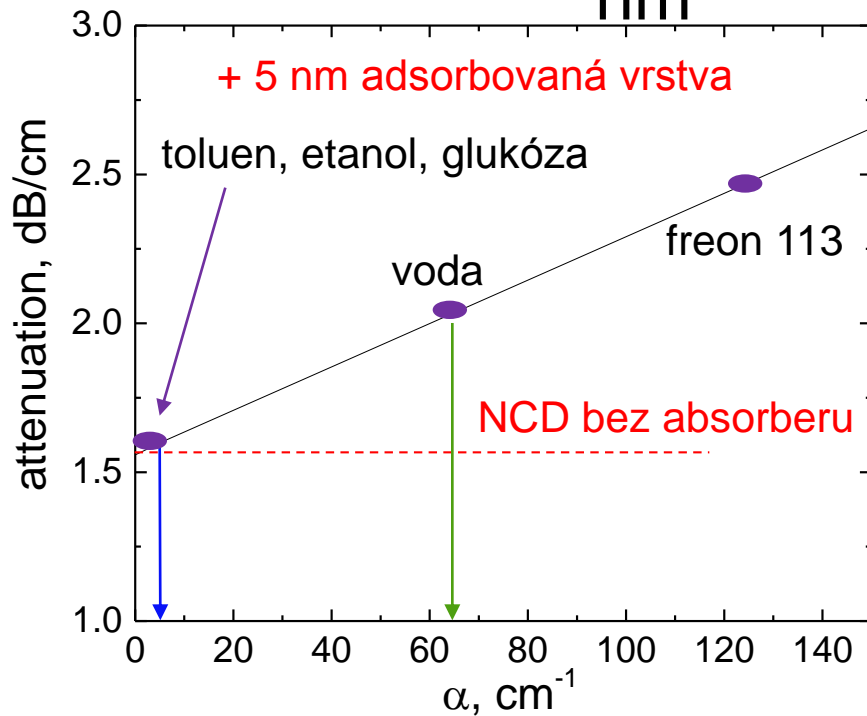
$h_{Si} = 280$ nm, TE_0 mód



- silně závislé na λ
- absorpce v NCD ovlivňuje šíření světla vlnovodem

Výsledky simulací– s adsorbovanou vrstvou

$$h_{NCD} = 50 \text{ nm}, \lambda = 2000 \text{ nm}$$



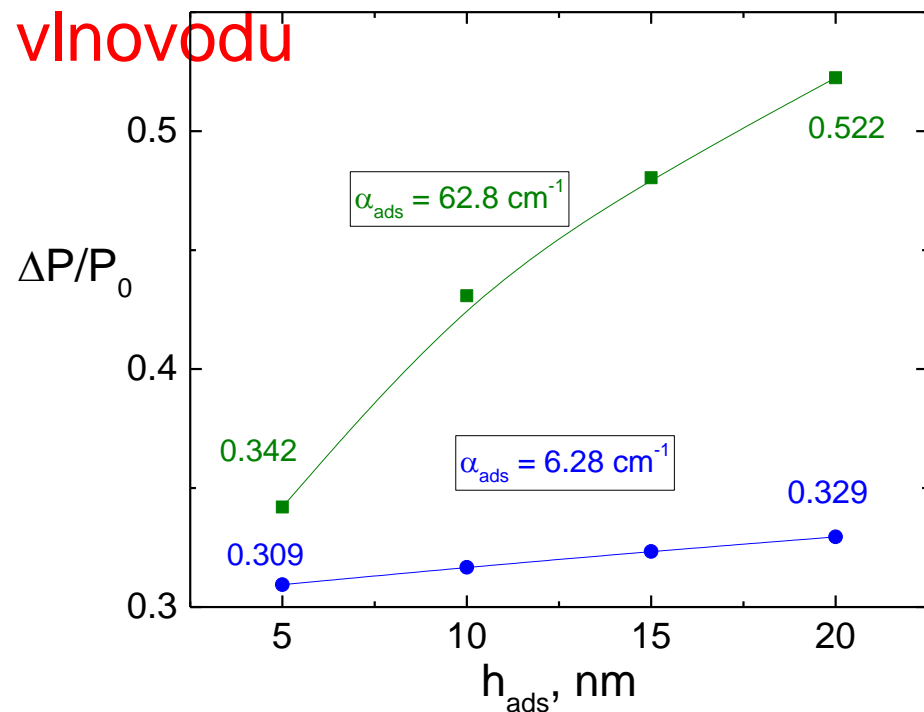
směrnice $\propto \alpha_{ads}$

□ vliv h_{abs}/h_{NCD}

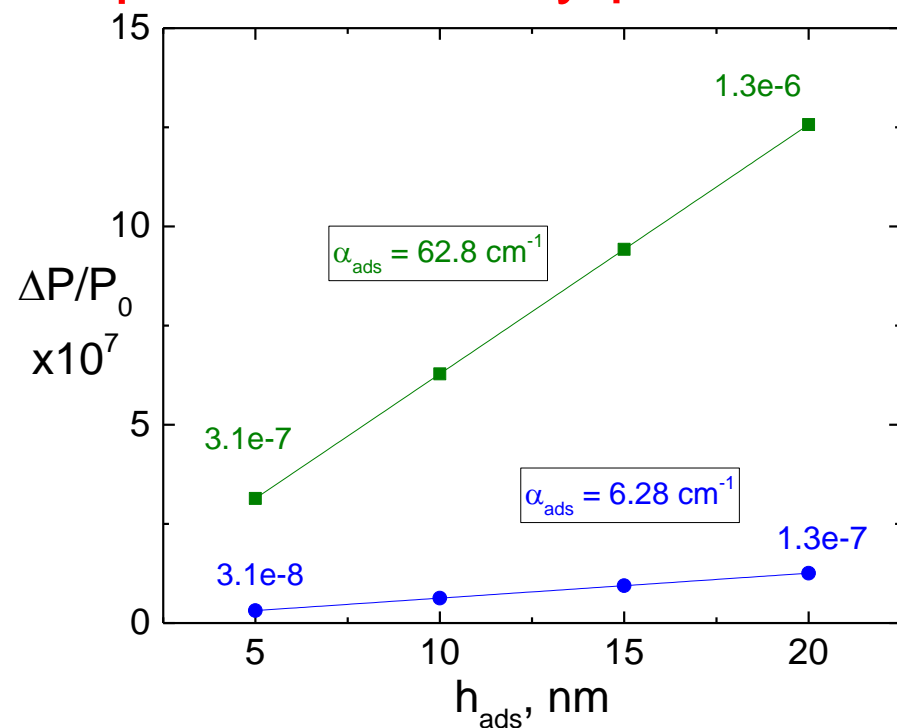
□ citlivost lze naladit délkou osvětlené části vlnovodu

Výsledky simulací – monitorování adsorpce

pokles intenzity na 1 cm vlnovodu



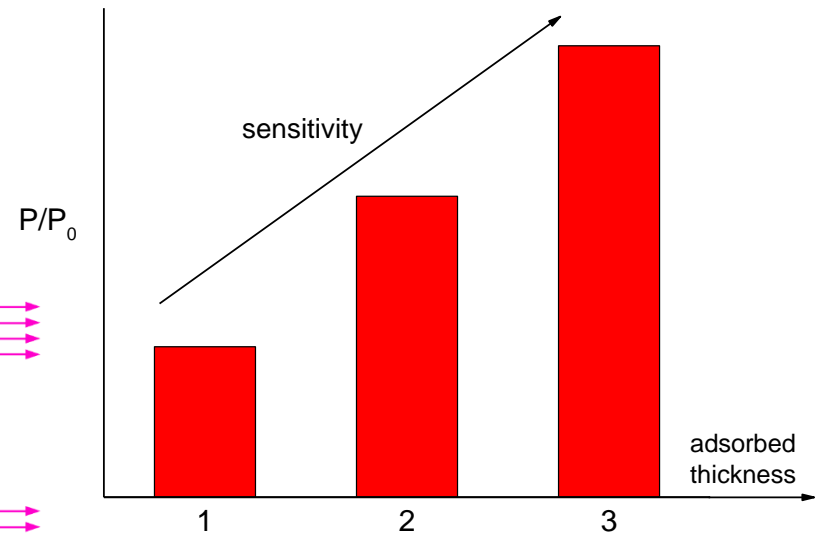
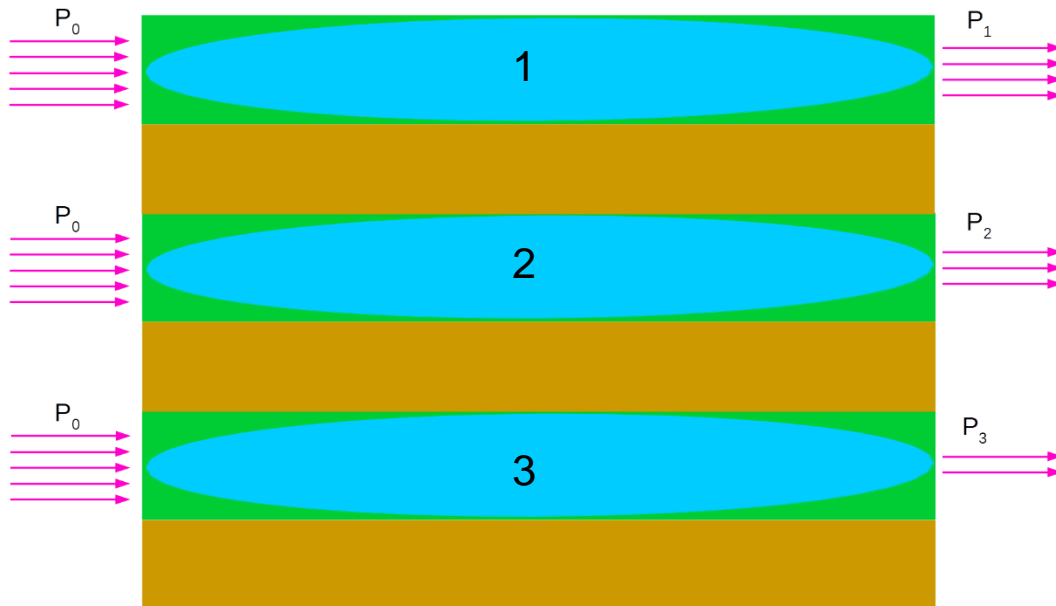
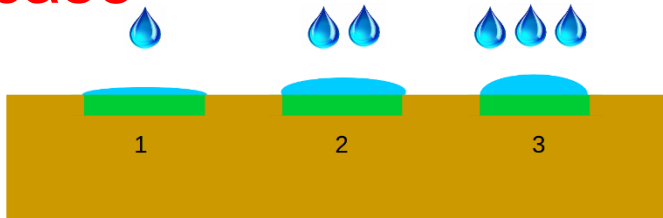
pokles intenzity při transmis



□ o několik řádů vyšší citlivost než transmisní spektrometrie

Výsledky simulací – monitor adsorpce

rychlý monitoring a řízení adsorpce v reálném čase



Závěr

- šíření světla planárním vlnovodem s absorpcí v krycí vrstvě vyřešeno FEM simulacemi ve 2D
- vysoce citlivý monitor adsorpce NCD/a-Si:H POWG v IČ oblasti je možný
- možnosti rozšíření výpočtů:
 - ▣ 3D geometrie
 - ▣ navázání a vyvázání světla
 - ▣ vliv rozptylu na hrubém rozhraní ?

Poděkování

Grantová agentura ČR, projekt č. 14-05053S.

Zdeněk Remeš
Václav Prajzler

remes@fzu.cz
prajzler@fzu.cz

Hledáme

NOVÉHO SPECIALISTU PRO FEM SIMULACE

- perspektivní obor
- bohatá mezioborová spolupráce v ČR i se zahraničím
- grantové, bilaterální, mezinárodní projekty

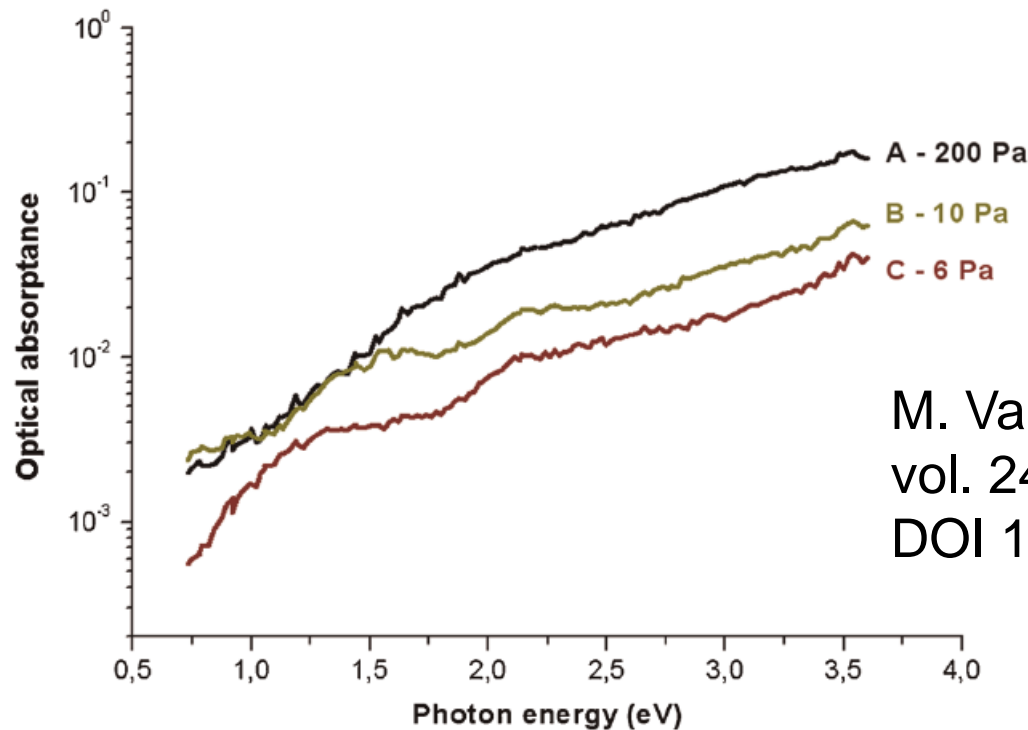
jirasek@fzu.cz

tel. 220 318 482

NCD for photonics – optical properties

□ Nanocrystalline diamond films (NCD)

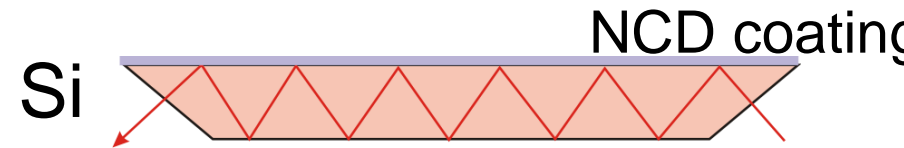
Optical absorption: sp^2 carbon & deposition



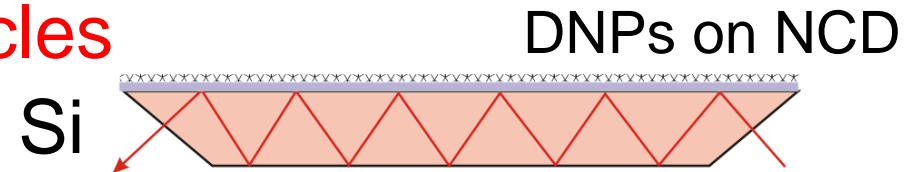
M. Varga *et al*, Phys. Status Solidi B
vol. 249, No. 12, 2635–2639 (2012)
DOI 10.1002/pssb.201200154

NCD for photonics – optical elements

ATR FTIR spectroscopy

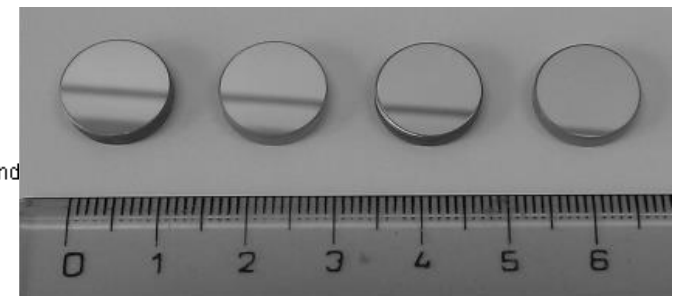
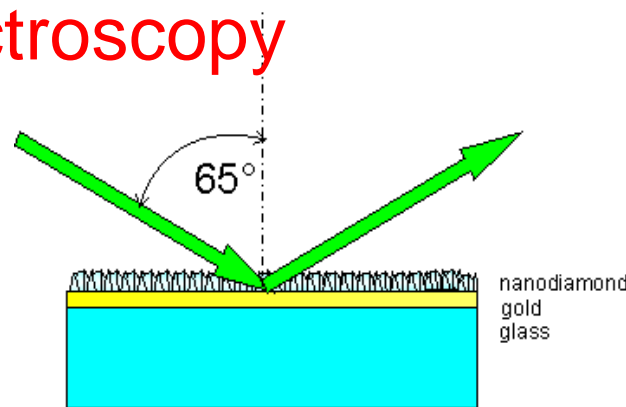


FTIR of diamond nanoparticles



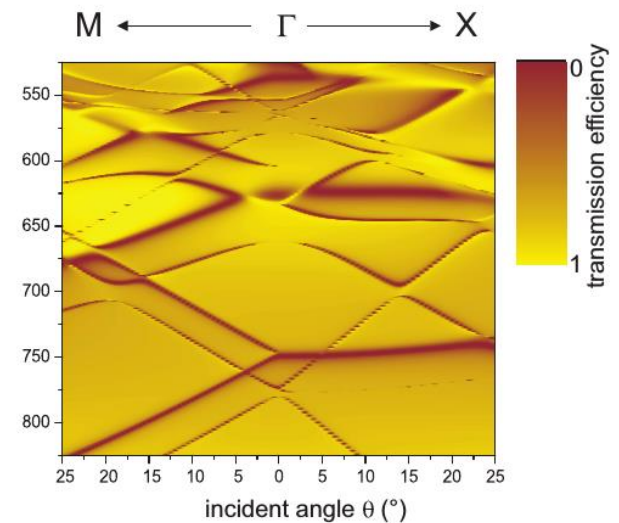
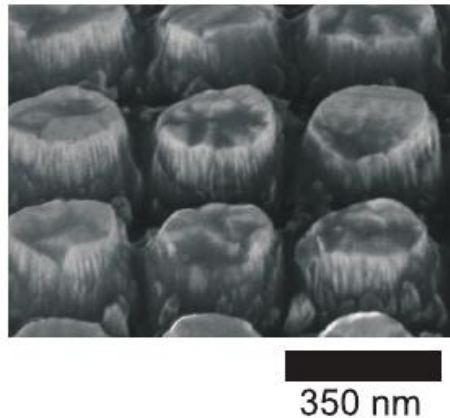
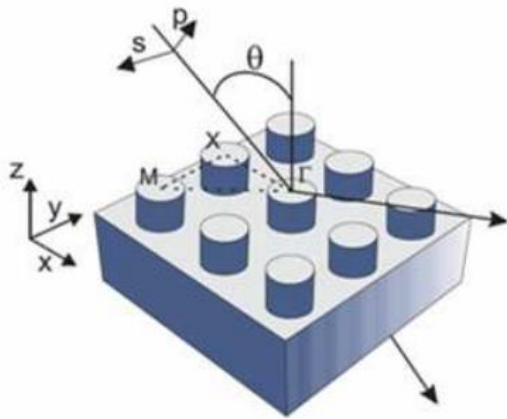
Remeš *et al.*, Appl. Surf. Sci. 270 (2013) 411 - 417.

GAR FTIR spectroscopy



Remeš *et al.*, Diam. Relat. Mater. 20 (2011) 882 - 885

CVD diamond for photonics – photonic crystal

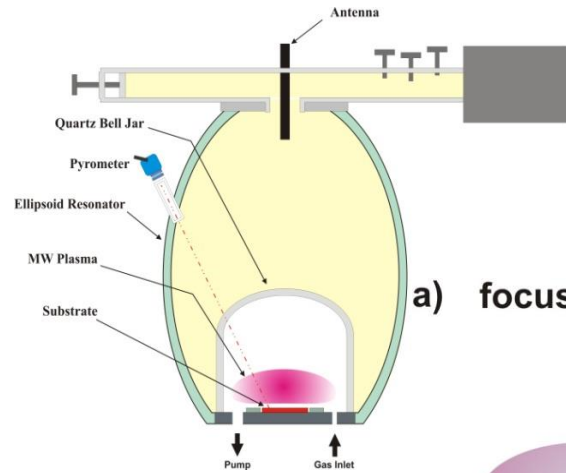


L. Ondič *et al.*, *Scient. Rep.* 2:914 (2012), DOI: 10.1038/srep00914

- selected wavelengths couple and propagate along
- tunable by nano-structuring

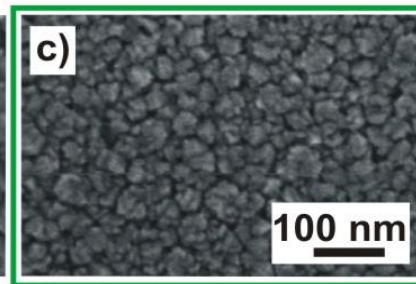
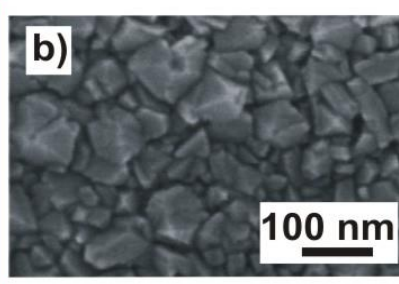
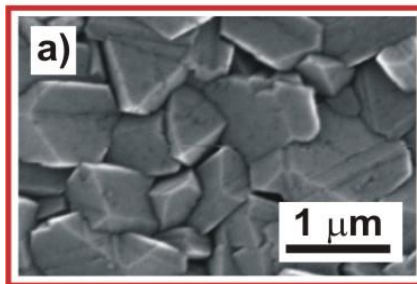
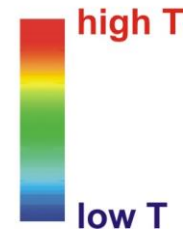
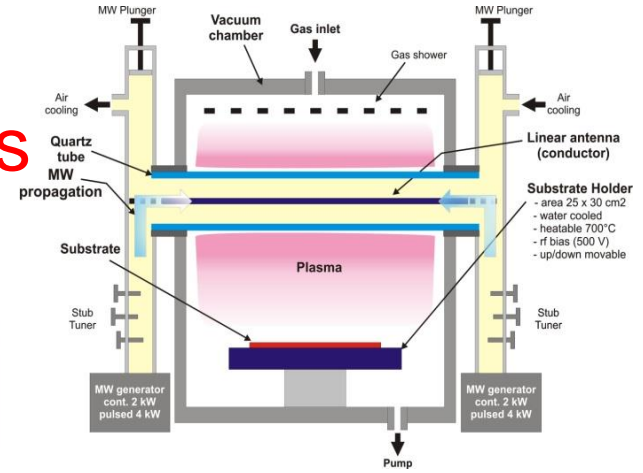
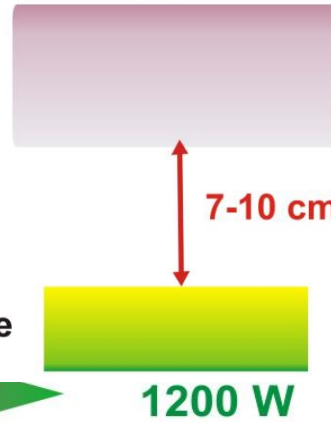
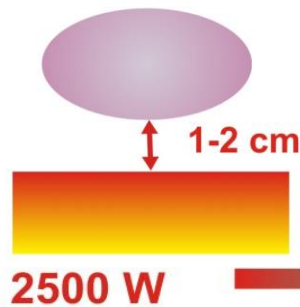
Nanocrystalline diamond films (NCD)

MW plasma reactors



a) focused plasma

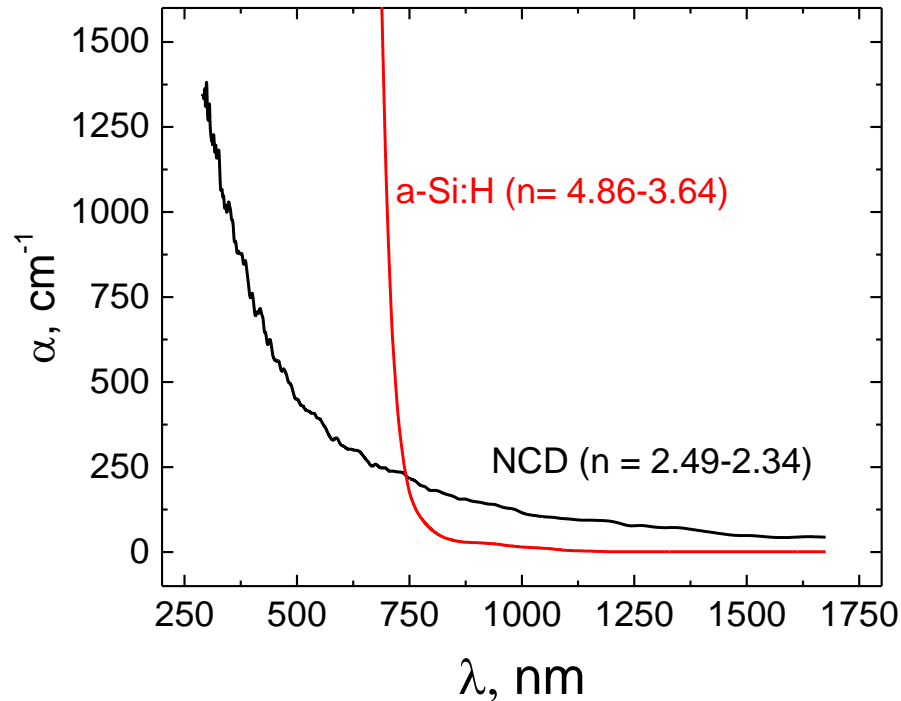
b) linear plasma



600 °C

250 °C

Optical absorption of NCD and a-Si:H



- absorption of a-Si:H in IR rather small
- NCD absorption in coating: influence on light propagation in POWG to be assessed by FEM simulation or measurement