Basic FEM modelling with COMSOL

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Software: COMSOL Multiphysics 5.6 (Build 280)

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Case 1: Optical property of thin-film stack

Task: Thin-film coatings are found in many optical devices for enhanced light transmission and reflection. A thin-film stack consisting of many layers of films of alternating refractive indices can even serve as a nearly perfect optical mirror. We refer to such a device a Bragg mirror/reflector/grating. In the following we model in COMSOL Multiphysics reflectance and transmittance spectra of a representative Bragg reflector.
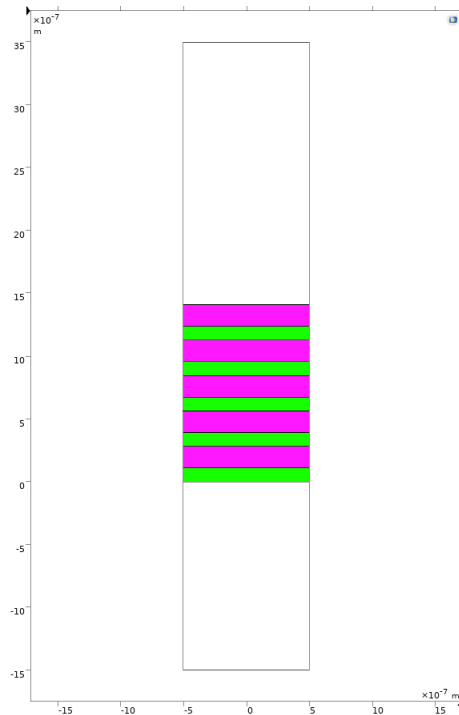

Fig. 1 Structure of a Bragg reflector. Coordinate: x→; y↑; z (out of paper).

Theory: This is a typical "frequency-domain" wave analysis where an input is specified to excite a material system within a computational domain. If both excitation and material system are invariant or have certain analytical dependence along one or more coordinate directions, one can often carry out simulation with reduced dimension. Here, since both plane wave and film stack are invariant along z direction, the problem is modelled in 2D.

Parameters and setup: Two dielectric materials are used to form the stack: a low-index SiO2 (magenta), and high-index TiO2 (green), with totally five periods. The two domains (white) above and below the stack are air. Both dielectric materials are assumed to have a constant refractive index: 1.45 for SiO2 and 2.28 for TiO2. When choosing the layer thicknesses, we used one quarter of light wavelength in the materials, with a targeted peak-reflection at free-space wavelength of 1um. Normal incident condition is examined: light is incident from the top domain boundary (port 1) with electric field polarized along z. Transmitted wave exits through the bottom domain boundary (port 2), and reflected wave exits through port. The left and right boundaries are periodic boundary conditions. Specific to the current setup, the periodic boundary condition simplifies to "perfect magnetic conductor" condition. Given the boundary conditions and light wavelength, COMSOL computes field distribution across the whole domain. Reflected and transmitted wave powers are calculated from field distribution at the top and bottom boundaries, which are built-in functions in COMSOL. Free-space wavelength range to be examined is 0.5-2um.

Finite-element analysis usually comprises of mainly four steps, namely **geometry** setup, **physics**/equation setup, **solver** setup, and **data analysis**. In the following, we choose to list the procedures in six steps in relation to how COMSOL is implemented.

Step A: Choose physics and study; set up parameters
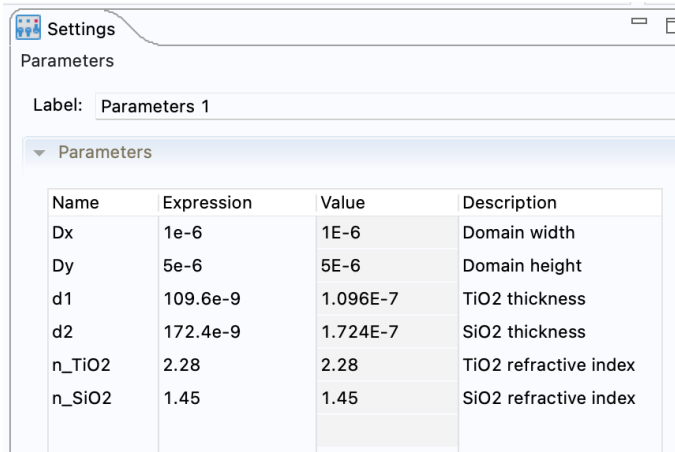
- Go to File→New. Click "Model Wizard". Click "2D".
- Under "Select Physics", expand "Optics", expand "Wave Optics".
- Select "Electromagnetic Waves, Frequency Domain (ewfd)". Click "Add". This item will be shown under "Added physics interfaces".
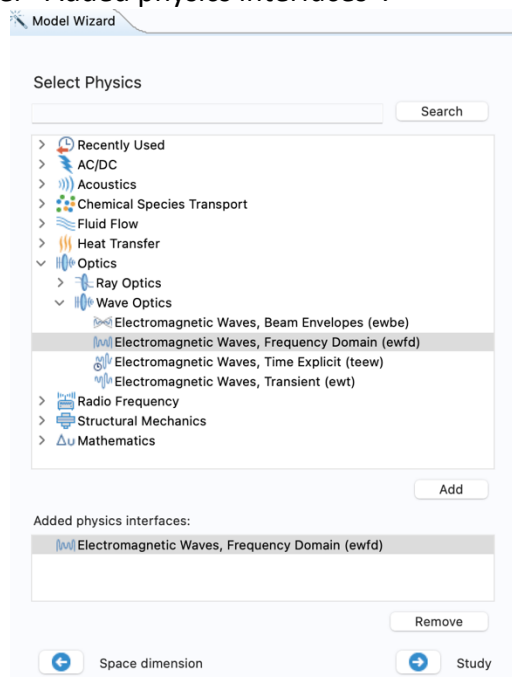
- Click "Study". Under "Preset Studies for Selected Physics interfaces", select "Wavelength Domain". Click "Done".
- You arrive at window below. The window is divided in general in three sub-windows: "Model Builder" on the left, "Settings" in the middle, and "Graphics" on the right. By default, you are asked to create geometry. Observe the units: "Length unit" is meter [m]; "Angular unit" is "Degrees".
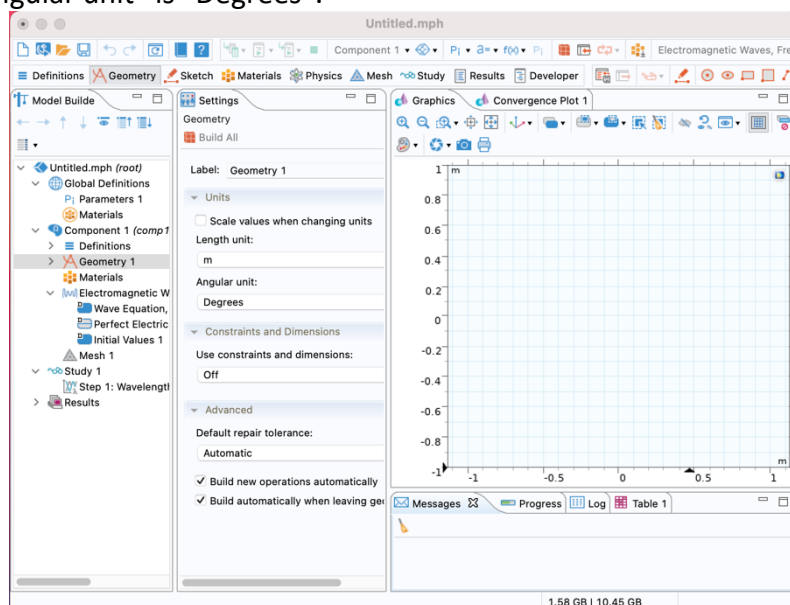
- Instead of editing "Geometry", we choose to set up "Parameters" first. Under "Model Builder" tree, select "Parameters 1". A table appears in the middle sub-window. Type in "Name" and "Expression" row by row according to screenshot below. These parameters are later used in setting up the model, both geometry and physics. "Description" serves as comment, which is not a must but helps to understand meaning of each parameter.
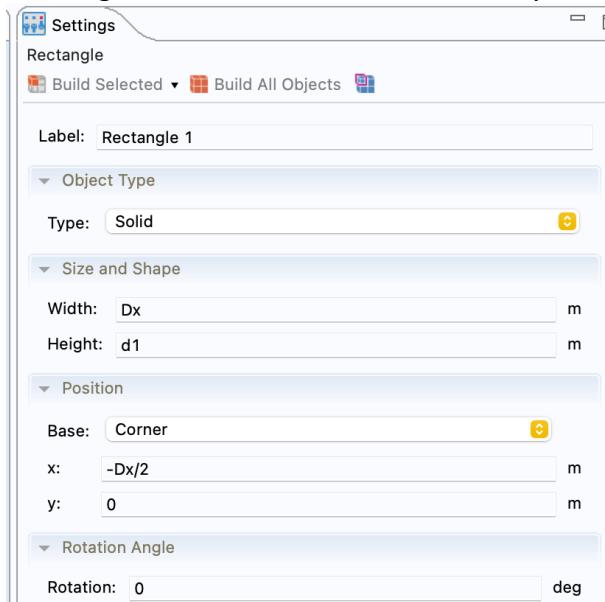

Step B: Build geometry

- Under "Model Builder", select "Geometry 1", and then right-click on it. Choose "Rectangle". An item "Rectangle 1 (r1)" will appear under "Geometry 1". In the middle sub-window "Settings", type in values according to the following under "Size and Shape" as well as "Position" fields. After clicking "Build Selected", a rectangle will be drawn on the right sub-window. This is essentially a TiO2 layer.

- We continue with a SiO2 layer. Right-click on "Geometry 1", and choose "Rectangle". This puts in "Rectangle 2 (r2)" under "Geometry 1". Under "Settings", assign the following parameters to the rectangle. After clicking "Build Selected", another rectangle will be drawn above the previous one. Tips: If the geometry is drawn beyond the plotted area in the right sub-window, one can always click on "Zoom extents" tool just above the plot to reveal the whole geometry.

Settings

Rectangle

Build Selected ▾ ▪ Build All Objects

Label: Rectangle 2

▾ Object Type

Type: Solid

▾ Size and Shape

Width: Dx   m
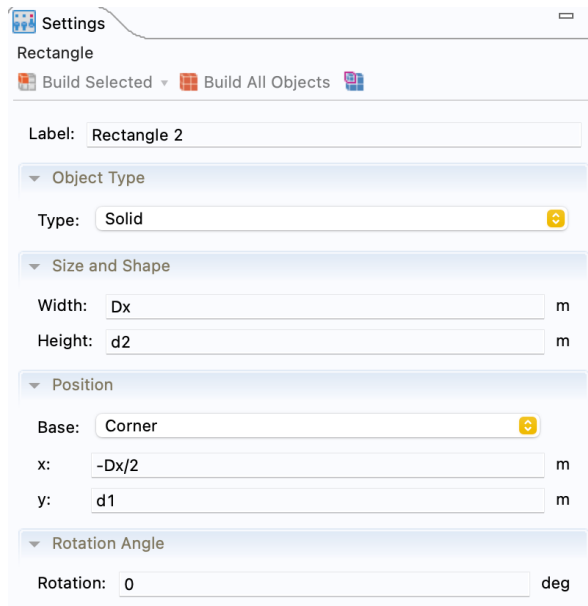Height: d2   m

▾ Position

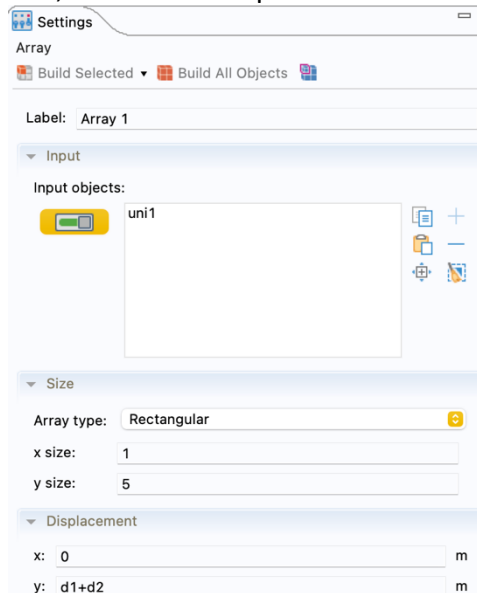Base: Corner

x: $-Dx/2$ m
y: d1   m

▾ Rotation Angle

Rotation: 0   deg

We have finished building one period of the grating. One can continue to build the rest four periods in the similar manner; but we can take a short-cut. We do this by combining the two layers into a single unit and use the unit as a basis to build a 1x5 array.

- Right-click "Geometry 1", and under "Booleans and Partitions" select "Union". Under "Settings", put in two rectangles into "input objects" by simply clicking on them in the right sub-window. Click "Build Selected".
- Right-click "Geometry 1", and under "Transforms" selected "Array". Under "Settings", put in the union (named "uni1") into the "input objects" simply by clicking on the union, and specify the rest parameters for the array as follows. After clicking "Build Selected", one obtains 5 periods of the bi-layers.

Settings

Array

Build Selected ▾ ▪ Build All Objects

Label: Array 1

▾ Input

Input objects:

uni1

▾ Size

Array type: Rectangular

x size: 1
y size: 5

▾ Displacement

x: 0   m
y: d1+d2   m

- Finally, one defines the simulation domain by creating a rectangle enclosing the film stack, which will create the air domains above and below the stack at the same time. Right-click "Geometry 1" and select "Rectangle", and under "Settings" enter the following parameters. Click "Build Selected" and then "Zoom Extents" to observe the whole geometry (as in Fig. 1, not in color though).
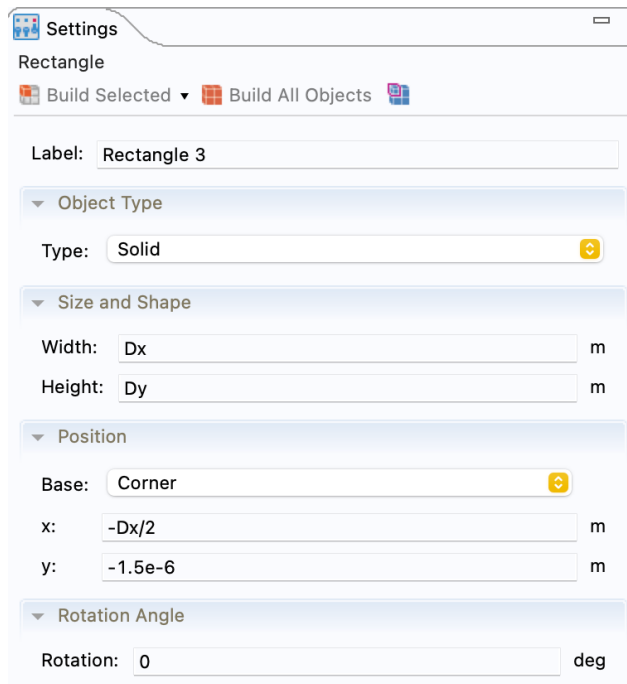
## Step C: Assign materials

We need three materials, TiO2, SiO2, and air. For optics, the only relevant physical parameter is refractive index. In this case study we deal with lossless materials. Therefore, the refractive indices are real numbers.

- In "Model Builder" tree, under "Component 1 (comp1)", select "Materials" and then right-click on it. In the pop-up context menu, choose "Blank Material". A new material named by default "Material 1 (mat1)" is created under "Materials". In "Setting" sub-window, change "Label" to "TiO2". By default, all sub-domains are assigned with this material, which is of course not the case. Keep only the desired TiO2 layers by getting rid of the SiO2 and Air layers (simply by clicking on them in the plot). In the "Material Contents" table, enter "n_TiO2" in "Value" column for "Refractive index, real part".
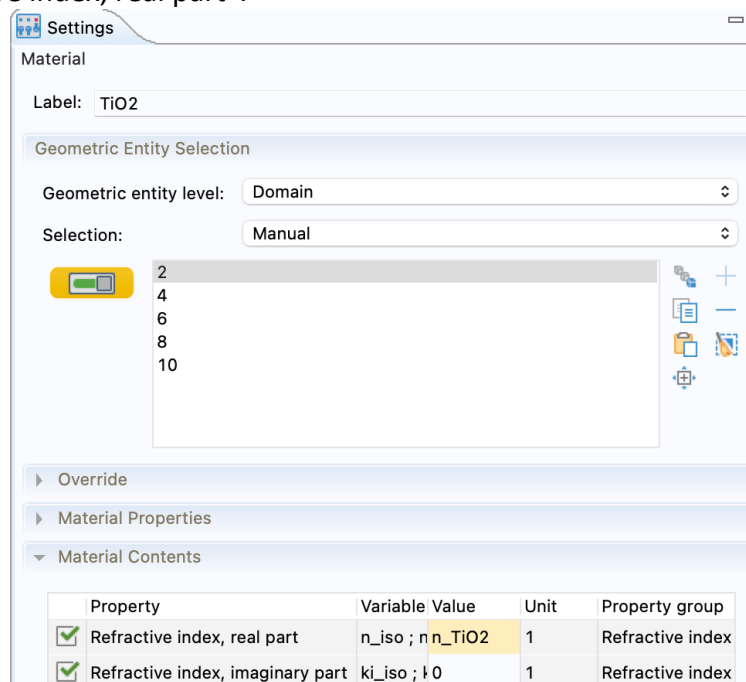
- Repeat the above for the SiO2 layers and Air layers. See screenshots below.

SiO2

Air
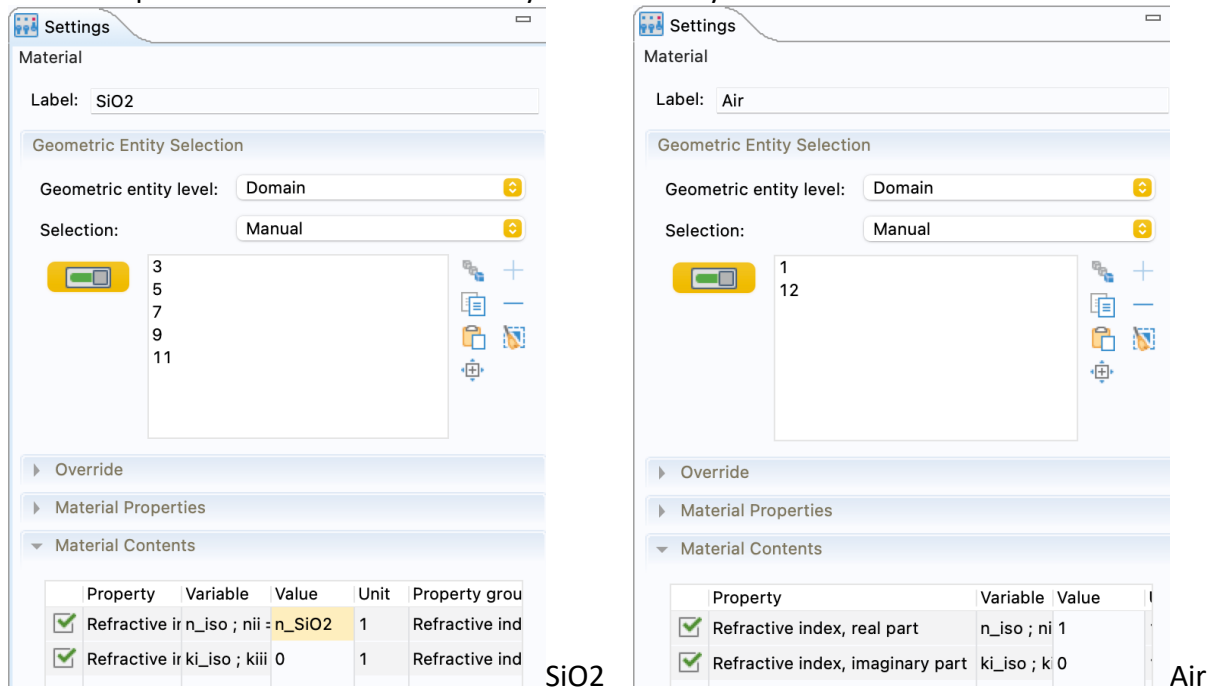
Step D: Define boundary conditions

When choosing "Physics and Study" we have asked COMSOL to use the right equation across the whole computational domain. However, it is almost always the case that one has to define some extra physics-related details before the model setup is complete. Usually, these are boundary conditions. Physically, these correspond to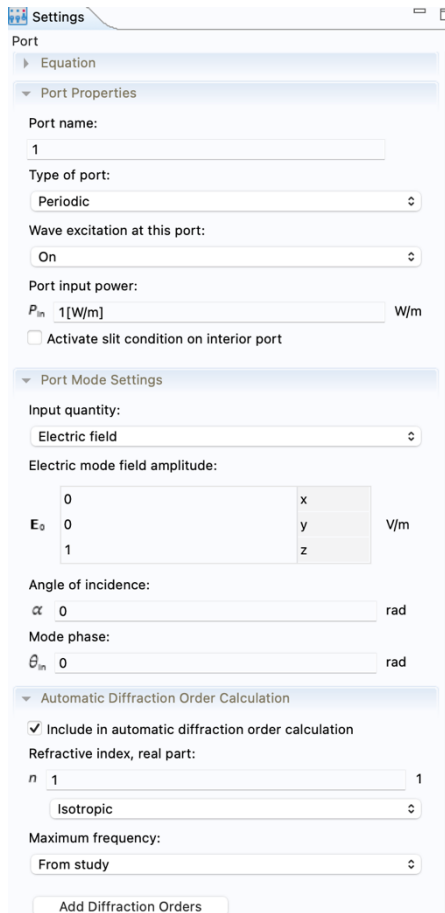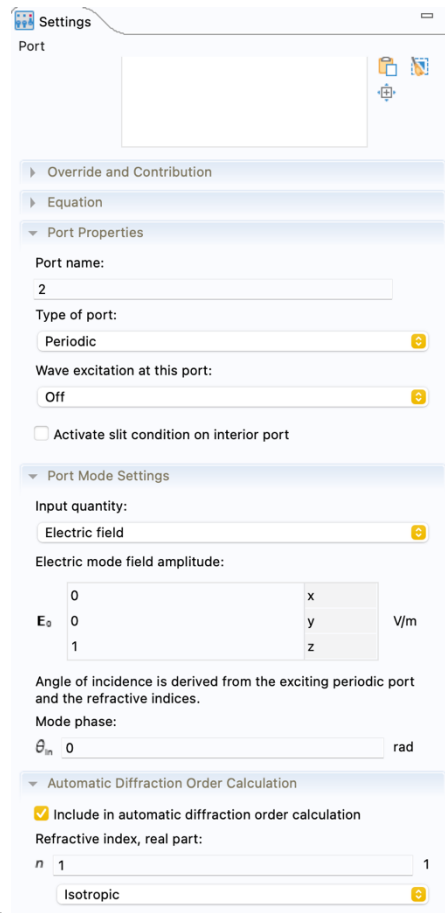, e.g., how the domain is excited, how wave interacts with the boundaries (reflecting or transmitting), or if any boundary is a symmetry axis of some "complete" model. In the latter case, one can use a small domain to model a huge domain by making use of its symmetry.

- First we define incident wave by defining a port. Under "Component 1 (comp1)", select "Electromagnetic Waves, Frequency Domain", and right-click on it. In the pop-up context menu, choose "Port". This will add "Port 1" under "Electromagnetic Waves, Frequency Domain".
- In the plot, click the topmost boundary. This will add boundary "25" into the table under "Boundary Selection" in the "Settings" sub-window.
- Down below in "Settings", set up "Port Properties", "Port Mode Settings" according to screenshot below. Note that the port is of type "Periodic" with normal plane-wave incidence whose E-field is polarized along z. Effectively, we are trying to model a thin-film with infinite area excited by a plane wave! The domain width Dx can in fact be set to any value ($Dx = 1\mu$m used in this model). In case you wonder whether we shall consider the x-coordinate at all: right, we can actually solve the given problem by considering just the y-coordinate. A 2D COMSOL modelling overkills.
- Create another port for the bottom boundary. Under "Component 1 (comp1)", select "Electromagnetic Waves, Frequency Domain", and right-click on it. In the pop-up context menu, choose "Port". This will add "Port 2" under "Electromagnetic Waves, Frequency Domain". In "Settings", set up "Port Properties", "Port Mode Settings" according to screenshot below

Port 1

Settings
Port

▶ Equation

▼ Port Properties

Port name:
1

Type of port:
Periodic

Wave excitation at this port:
On

Port input power:
P_{in} 1[W/m] W/m

☐ Activate slit condition on interior port

▼ Port Mode Settings

Input quantity:
Electric field

Electric mode field amplitude:

E_0
0	x
0	y
1	z

V/m

Angle of incidence:
α 0 rad

Mode phase:
θ_{in} 0 rad

▼ Automatic Diffraction Order Calculation

☑ Include in automatic diffraction order calculation

Refractive index, real part:
n 1   1

Isotropic

Maximum frequency:
From study

Add Diffraction Orders

Port 2

Settings
Port

▶ Override and Contribution

▶ Equation

▼ Port Properties

Port name:
2

Type of port:
Periodic

Wave excitation at this port:
Off

☐ Activate slit condition on interior port

▼ Port Mode Settings

Input quantity:
Electric field

Electric mode field amplitude:

E_0
0	x
0	y
1	z

V/m

Angle of incidence is derived from the exciting periodic port and the refractive indices.

Mode phase:
θ_{in} 0 rad

▼ Automatic Diffraction Order Calculation

☑ Include in automatic diffraction order calculation

Refractive index, real part:
n 1   1

Isotropic

- Finally, let COMSOL know that the domain is part of an actual domain we wanted to simulate by setting the left and right boundaries as a kind of periodic boundaries. As mentioned, particularly for the incidence angle and polarization used, one can definite the boundaries as "Perfect Magnetic Conductors". Under "Component 1 (comp1)", select "Electromagnetic Waves, Frequency Domain", and right-click on it. In the pop-up context menu, choose "Perfect Magnetic Conductor". This will add "Perfect Magnetic Conductor 1" under "Electromagnetic Waves, Frequency Domain". Click in the plot on the left and right boundaries (all sections), which will add them into the table under "Boundary Selection" in "Settings".

Step E: Mesh

FEM generally uses unstructured mesh (e.g. triangular mesh in 2D cases), which implies the mesh resolution can be adapted to one's need. The general rule-of-thumb is to let mesh size (triangular edge size) to be 1/5 of wavelength in medium under consideration. In this case study we are going to compute reflectance and transmittance spectra for free-space wavelength range [0.5, 2]um. From the minimum wavelength, we estimate mesh size should be roughly 50, 70, 100nm in TiO2, SiO2, and air regions, respectively.

- In "Model Builder", select "Mesh 1" and right-click on it. In the pop-up context menu, select "Size". This will generate "Size" and "Size 1" items under "Mesh 1".
- In "Model Builder", click "Size" item. In the middle "Settings" sub-window, select "Custom" under "Element Size". Then type "100e-9"m for "Maximum element size". This sets a global upper limit for triangular edge size across the whole domain.
- In "Model Builder", click "Size 1" item. In the middle "Settings" sub-window, make sure to select "Domain" for "Geometric entity level", and "Selection" is "Manual". In

the table below, put in domains corresponding to the TiO2 layers. Enable "Custom" for "Element Size" and set "Maximum element size" to "70e-9"m. See screenshot below.

- Repeat the above step and create another "Size" called "Size 2" under "Mesh 1". Set up according to the screenshot below (right). It controls maximum mesh size for SiO2 layers.
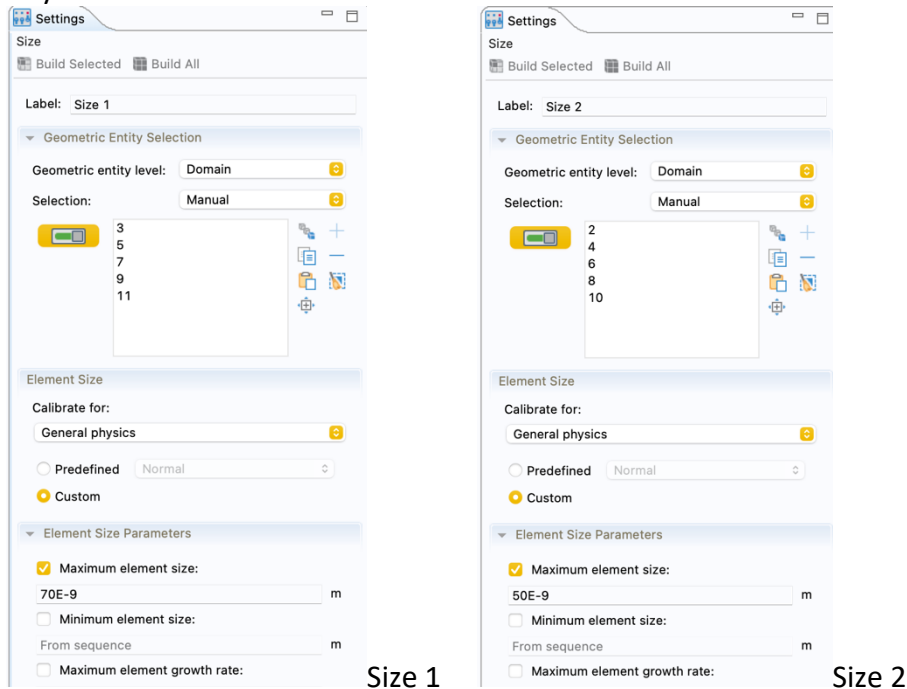
Size 1   Size 2

- In "Model Builder", select "Mesh 1" and right-click on it. In the pop-up context menu, select "Free Triangular". "Free Triangular 1" will then appear under "Mesh 1". Click "Build All" to ask COMSOL to mesh the domain using triangular mesh.

Step F: Solve and analyze data

- In "Model Builder", under "Study 1", select "Step 1: Wavelength Domain". In the middle "Settings" sub-window. Set the wavelength according to the following.
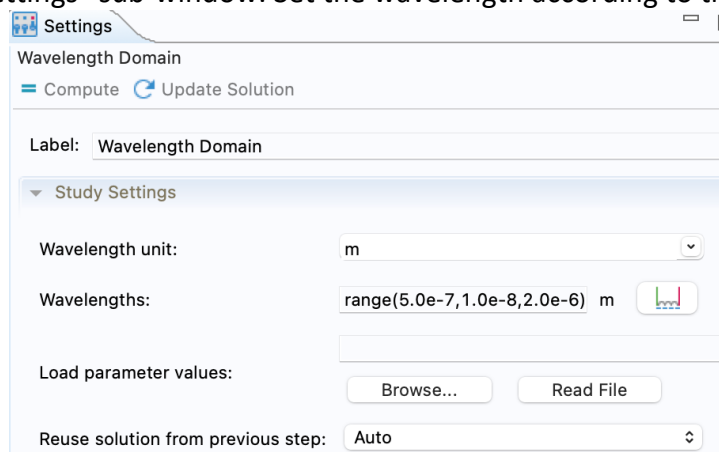

To avoid confusion, use "m" for "Wavelength unit". One may type in directly the range for "Wavelengths". Otherwise click on the symbol to the right and use the pop-up window to create the range. It is from 500nm to 2000nm with a step of 10nm. This effectively means COMSOL will repeatedly calculate reflectance and transmittance 151 times, each time with a different incident wavelength.

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- Click "Compute" to start computation. On a good computer the calculation finishes in 10-20 seconds. It is good time to take a coffee in case you have a slow computer.
- By default, COMSOL will show you a plot of electric field (norm) at the last wavelength computed, shown below. In "Model Builder", "Electric Field (ewfd)" is highlighted. In the middle "Settings" window, one can choose another wavelength under "Parameter value (lambda0 (m))" field to examine corresponding field distribution. In this way, one can visually inspect when the film stack is transmitting, when is not (reflecting). One can also choose which field to be plotted by expanding "Electric Field (ewfd)" item in "Model Builder". Select "Surface 1", and in "Settings", replace expression "ewfd.normE" by "ewfd.Hx" to see the Hx field plot.

lambda0(151)=2E-6 m Surface: Electric field norm (V/m)
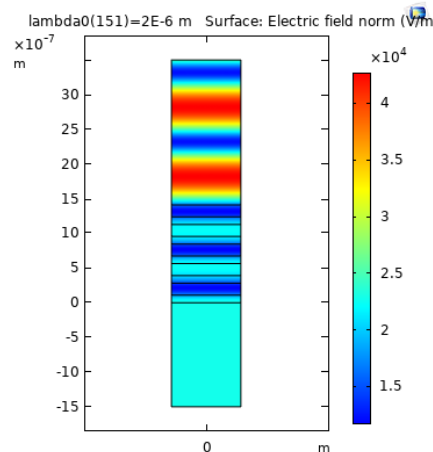
- More accurately we want reflectance and transmittance spectra. To obtain this we create a 1D line plot. In "Model Builder", select "Results" and then right-click on it. In the pop-up context menu, select "1D Plot Group". In "Settings", change its label from the default "1D Plot Group 1" to "Reflectance and Transmittance". Under "Plot Settings", type in x- and y-axis labels as "Wavelength [m]" and "Reflectance, Transmittance", respectively.
- In "Model Builder", right-click on "Reflectance and Transmittance". In the pop-up context menu, choose "Global". "Global 1" is created in the model tree. In "Settings", under "y-Axis Data", type in the following information to the table.
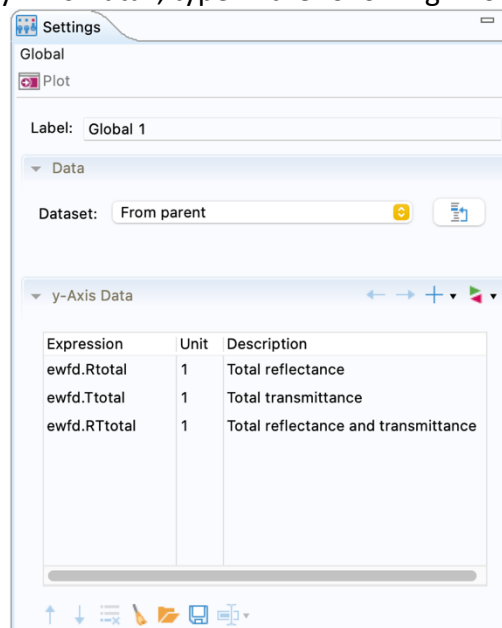
- Click "Plot". One obtains transmittance, reflectance spectra, as well sum of the two. One should be relieved to see that peak reflection occurs around 1um, as well as that sum of reflectance and transmittance is always (close to) unity.
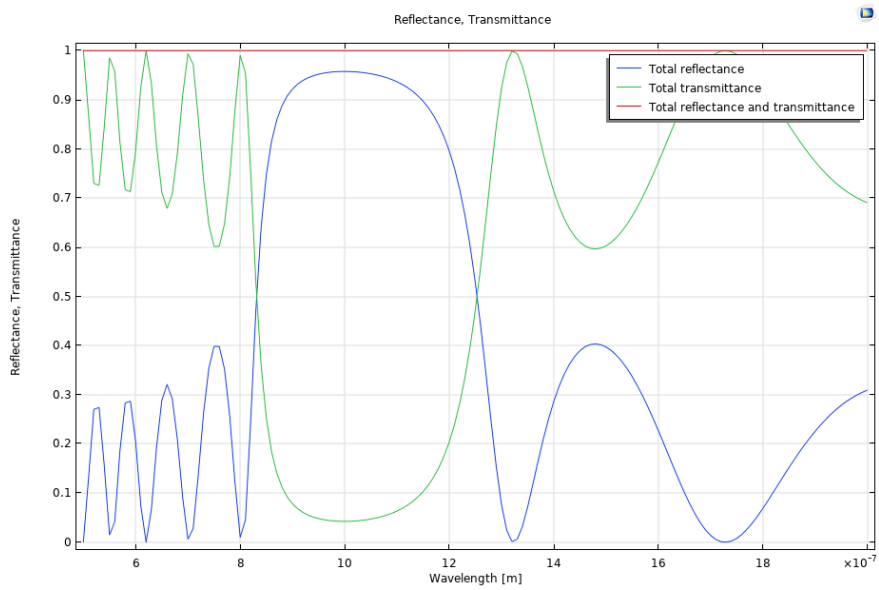
Case 2: Cut-off of SU-8 waveguide

Task: This case study is to calculate with COMSOL Multiphysics guided modes in a SU-8 polymer waveguide and to find out its cut-off wavelength for single-mode operation. Essentially, this case study is applicable for any regular or uniform waveguide, i.e. waveguide whose cross-section is the same along wave-guiding direction.

Theory: This problem belongs to the so-called "eigen-mode" analysis. No excitation is needed in such a study. FEM will find out natural "resonant" mode(s) of a given physical system. For waveguiding problems, input includes geometry, material composition, and frequency or free-space wavelength λ_0. The desired output is modal propagation constant(s) β or eigenvalue(s), and of course the modal field distribution(s) or eigenvector(s). The relation between frequency against propagation constant is commonly referred to dispersion relation. In optics community, one often chooses to plot the dispersion relation using λ_0 and effective mode index ($n_{\text{eff}} = \beta/k_0$).
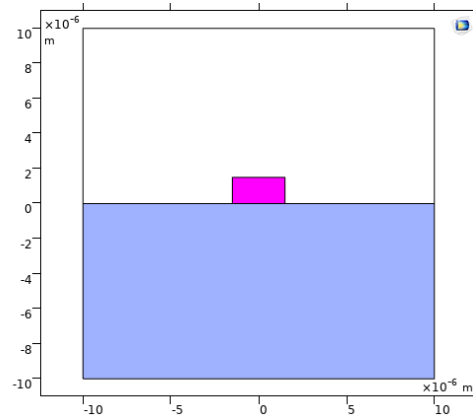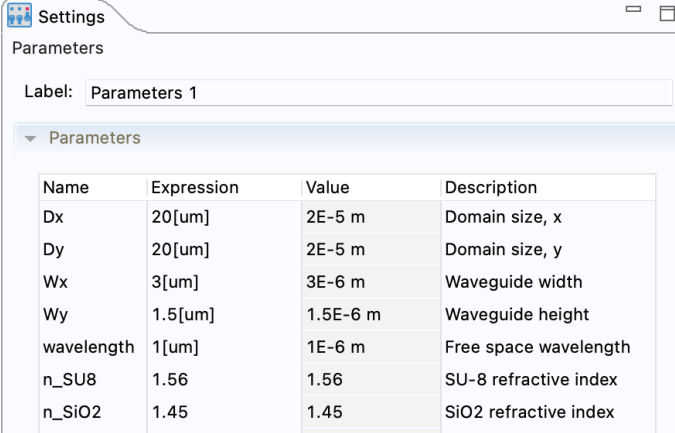

Ideally, one shall use infinite cross-section for such mode analysis. However, in COMSOL, one has to limit simulation domain to a finite size. If the domain used is large enough so that field of the interested mode decays to a negligible value, the condition at the outmost domain boundary is not that all important. Some smart researchers have come up with ideas to use the outermost domain boundary or a thin boundary layer to emulate an open-boundary condition. That is, wave field extending outwards, propagating or decaying, from the domain, will experience no reflection. People refer to such conditions as "transparent" or "scattering" or "open" boundary condition. The most popular implementation uses a boundary layer, called "perfectly matched layer" or PML to achieve such effect. Wave impinging onto such a layer experience no reflection regardless of wavelength, incident angle or polarization. However, we will not touch PML in this case study, but focus on simpler "Scattering boundary condition".

Parameters and setup: As shown in the cross-section plot, the SU-8 waveguide (magenta) is sitting on top of SiO2 substrate (blue). The half domain above (white) is simply air. Refractive indices for SU-8 and SiO2 are assumed to frequency-independent, valued at 1.56 and 1.45, respectively. The SU-8 waveguide has width of 3um and height 1.5um. I have made some preliminary effort to make sure the waveguide is single-mode at 1.55um free-space wavelength, and multi-mode at 1.0um free-space wavelength. We would like to find out more clearly at which wavelength it will become single-mode. We will use sweep in COMSOL to repeatedly calculate low-order modes in the waveguide, each time with a different wavelength (between 1um to 1.6um). A plot of the effective modal indices with respect to wavelength can reveal the cut-off wavelength.

We follow the same six steps in the previous case study.
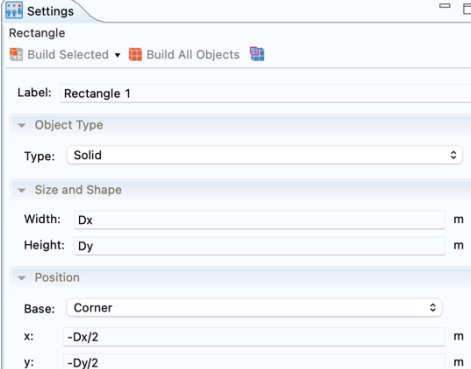
Step A: Choose physics and study; set up parameters

- Go to File→New. Click "Model Wizard". Click "2D".
- Under "Select Physics", expand "Optics", expand "Wave Optics".
- Select "Electromagnetic Waves, Frequency Domain (ewfd)". Click "Add". This item will be shown under "Added physics interfaces".
- Click "Study". Under "Preset Studies for Selected Physics interfaces", select "Mode Analysis". Click "Done".
- In the subsequent window, by default, you are asked to create geometry. Observe the units: "Length unit" is meter [m]; "Angular unit" is "Degrees".
- Under "Model Builder" tree, select "Parameters 1". Type in parameters according to the screenshot below.

Settings

Parameters

Label: Parameters 1

Parameters

Name	Expression	Value	Description
Dx	20[um]	2E-5 m	Domain size, x
Dy	20[um]	2E-5 m	Domain size, y
Wx	3[um]	3E-6 m	Waveguide width
Wy	1.5[um]	1.5E-6 m	Waveguide height
wavelength	1[um]	1E-6 m	Free space wavelength
n_SU8	1.56	1.56	SU-8 refractive index
n_SiO2	1.45	1.45	SiO2 refractive index

Step B: Build geometry

- Select "Geometry 1", and then right-click on it. Choose "Rectangle". An item "Rectangle 1 (r1)" will appear under "Geometry 1". In the middle sub-window "Settings", type in values according to the following under "Size and Shape" as well as "Position" fields. After clicking "Build Selected", a rectangle will be drawn in the Graphics sub-window. This defines the simulation domain.

Settings

Rectangle

Build Selected ▾   Build All Objects

Label: Rectangle 1

Object Type

Type: Solid

Size and Shape

Width: Dx   m
Height: Dy   m

Position

Base: Corner

x: –Dx/2   m
y: –Dy/2   m

- Create another rectangle, called "Rectangle 2(r2)". Define it as follows. Width: Dx; Height: Dy/2; Base: Corner, with x=-Dx/2 and y=-Dy/2. Click "Build Selected". This builds the substrate.
- Create another rectangle, called "Rectangle 3(r3)". Define it as follows. Width: Wx; Height: Wy; Base: Corner, with x=-Wx/2 and y=0. Click "Build Selected". This builds the SU-8 waveguide.

Step C: Assign materials

We need three materials, Air, SU-8, and SiO2. PML layers' materials will be defined by COMSOL automatically. For optics, the only relevant physical parameter is refractive index. In this case study we deal with lossless materials. Therefore, the refractive indices are real numbers.

- In "Model Builder" tree, under "Component 1 (comp1)", select "Materials" and then right-click on it. In the pop-up context menu, choose "Blank Material". A new material named by default "Material 1 (mat1)" is created under "Materials". In "Setting" sub-window, change "Label" to "Air". By default, all sub-domains are assigned with this material, which is of course not the case. Keep only the desired Air domain by getting rid of the SU-8 and SiO2 domains (simply by clicking on them in the plot). In the "Material Contents" table, enter "1" in "Value" column for "Refractive index, real part". See screenshot below.
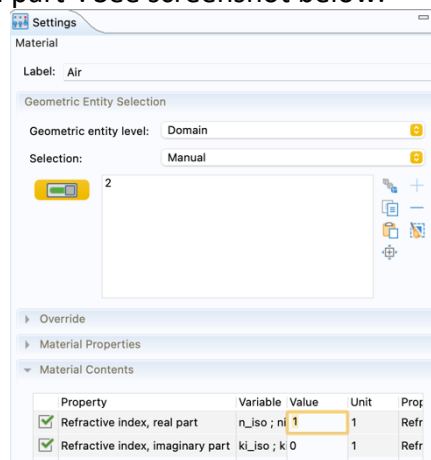
- Repeat the above for the SU-8 and SiO2 domains. Refer to screenshots below.
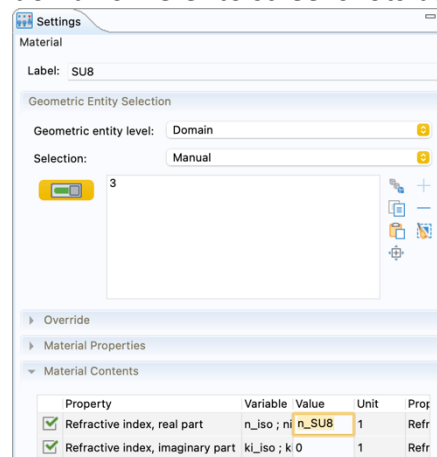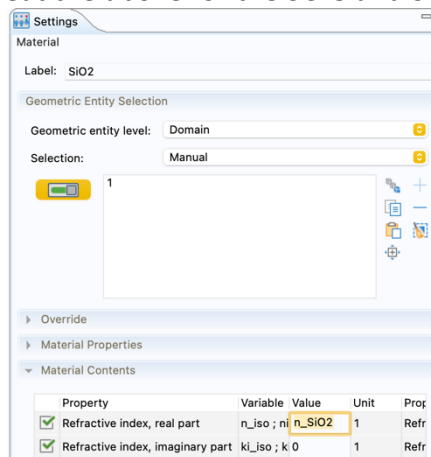
Step D: Define boundary conditions

As mentioned in "Theory", there is no need to define wave excitation for "Mode analysis". What needs attention is the outer domain boundary. If simulation domain is not large enough, there exists risk that mode field can reach the outermost domain boundary. Reflection by the outermost boundary can affect modal field distribution across the whole domain. To minimize this adverse effect, one can define the outermost boundary as "Scattering Boundary Condition".

- In "Model Builder", under "Component 1 (comp 1)", select "Electromagnetic Waves, Frequency Domain (ewfd)" and right-click on it. In the pop-up context menu, select "Scattering Boundary Condition". This will create "Scattering Boundary Condition 1" under the tree. Click in the plot the outer boundary lines (1, 2, 3, 5, 7, 11, 12) so they are added into "Boundary Selection" table in "Setting" sub-window.
- Further down in the "Settings", under "Scattered wave type", choose "Cylindrical wave". This is because we have put the waveguide core close to the domain center. Modal fields at the outer boundary will have more or less cylindrical wave front.

Step E: Mesh

- In "Model Builder", select "Mesh 1" and right-click on it. In the pop-up context menu, select "Size". This will generate "Size" and "Size 1" items under "Mesh 1".
- In "Model Builder", click "Size" item. In the middle "Settings" sub-window, select "Custom" under "Element Size". Then type "1e-6"m for "Maximum element size". This sets a global upper limit for triangular edge size across the whole domain.
- In "Model Builder", click "Size 1" item. In the middle "Settings" sub-window, make sure to select "Domain" for "Geometric entity level", and "Selection" is "Manual". In the table below, put in the SU-8 domain (3). Enable "Custom" for "Element Size" and set "Maximum element size" to "0.3e-6"m.
- Repeat the above step and create another "Size" called "Size 2" under "Mesh 1". In the middle "Settings" sub-window, make sure to select "Domain" for "Geometric entity level", and "Selection" is "Manual". In the table below, put in the SiO2 domain (1). Enable "Custom" for "Element Size" and set "Maximum element size" to "0.5e-6"m.
- In "Model Builder", select "Mesh 1" and right-click on it. In the pop-up context menu, select "Free Triangular". "Free Triangular 1" will then appear under "Mesh 1". Click "Build All" to ask COMSOL to mesh the domain using triangular mesh.

Step F: Solve and analyze data

- In "Model Builder", under "Study 1", select "Step 1: Mode Analysis". In the middle "Settings" sub-window. Set the parameters according to the following.
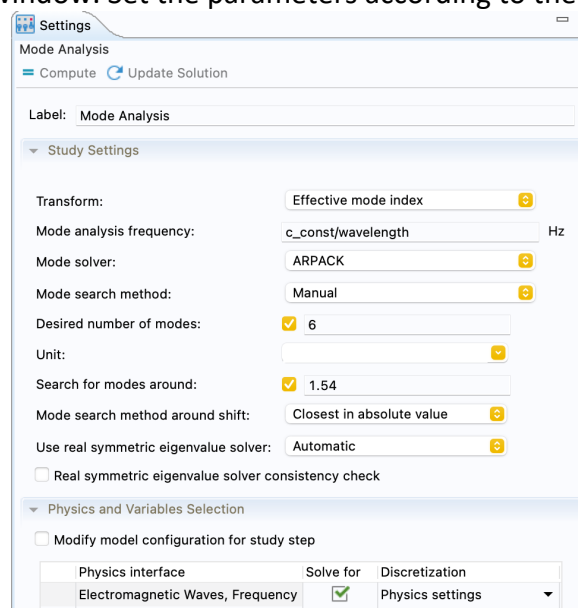

Note the way frequency is specified through "wavelength" parameter (free space wavelength, $1\mu m$). And we choose to search for 6 modes with "effective mode

index" around 1.54, which is a bit lower than the refractive index of waveguide core (SU-8), and higher than cladding index (SiO2 or Air).

- Click "Compute".
- By default, COMSOL will show the mode with smallest n_{eff}, which is a high-order mode. See screenshot below. Color scale is by default Electric field norm.
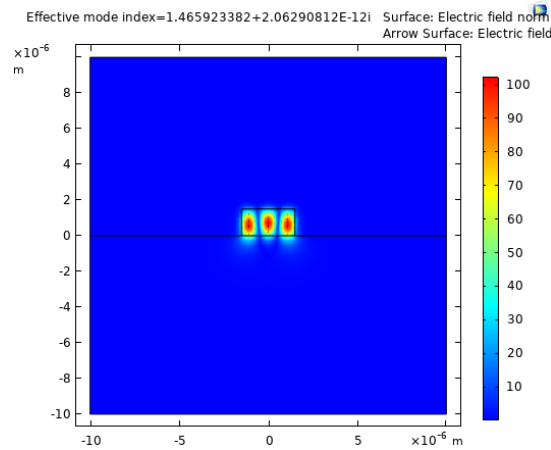

- While in "Model Builder" the item "Results/Electric Field (ewfd)" is selected, one can view one of the other 5 modes by choosing another "Effective mode index". The fundamental mode has often the largest n_{eff} value. Choose the last one (1.5297…) in the list, shown below. One plots the fundamental mode.
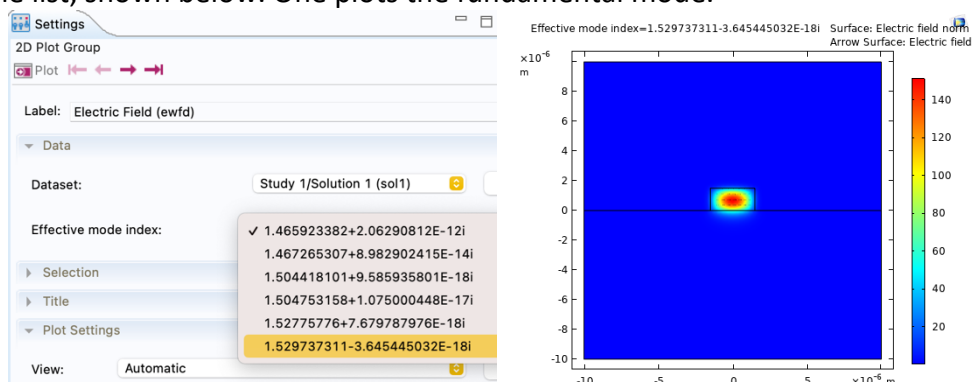
- To see polarization of the field: in "Model Builder", select "Electric Field (ewfd)" and right-click on it. In the pop-up context menu, choose "Arrow Surface". This will create an item "Arrow Surface 1" under "Electric Field (ewfd)". In the item's "Settings" sub-window, set up the parameters according to the screenshot below.
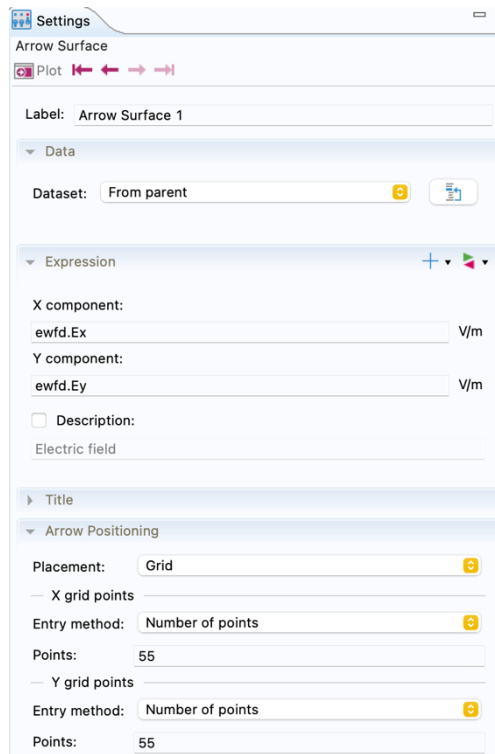
This will plot a vector electric field in the domain with 55x55 arrows. Such information is important because some modes may appear similar in terms of $|\boldsymbol{E}|$ but have different electric field components.

So far, we have successfully identified modes at $\lambda_0 = 1\mu$m. We would like to know at which wavelength the waveguide can become single-mode. This can be simulated through a parameter sweeping with respect to λ_0.

- In "Model Builder" tree, select "Study 1/Step 1: Mode Analysis". In "Settings", under "Study Extensions", enable "Auxiliary sweep". In the table below, click "+" sign, and from there choose "wavelength (Free space wavelength)". This will add it to the table under "Parameter name". Type in "Parameter value list" and "Parameter unit" according to the screenshot below.
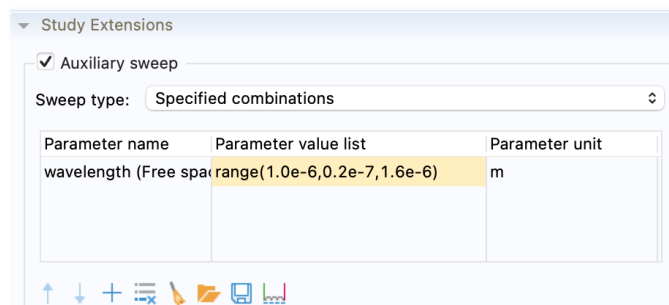

This will ask COMSOL to repeatedly calculate modes for wavelengths beginning at 1 μm and finishing at 1.6 μm, with 20 nm step size (total 31 calculations).
- Click on "Compute". It will take a couple of minutes or more before calculation finishes.
- To see the cut-off condition, we plot out the computed n_{eff} values with respect to λ_0, i.e. so-called dispersion curves. In "Model Builder", select "Results" and right-click on it. In the pop-up context menu, select "1D Plot Group". This will add and

item called "2D Plot Group 1" under the tree. In corresponding "Settings", change the label to "Modal dispersion", and type "x-axis label" as "Wavelength [m]" and "y-axis label" as "Effective mode index".

- Right-click on "Modal dispersion". In the pop-up context menu, select "Global". This will add "Global 1" item under "Modal dispersion". In the corresponding "Settings" sub-window, type in "ewfd.neff" under "Expression" in "y-Axis Data" table. See screenshot below (left). Further down in "Settings", set "x-Axis Data" as in the screenshot below (middle). Further down in "Settings", set "Color and Style" according to the screenshot below (right).
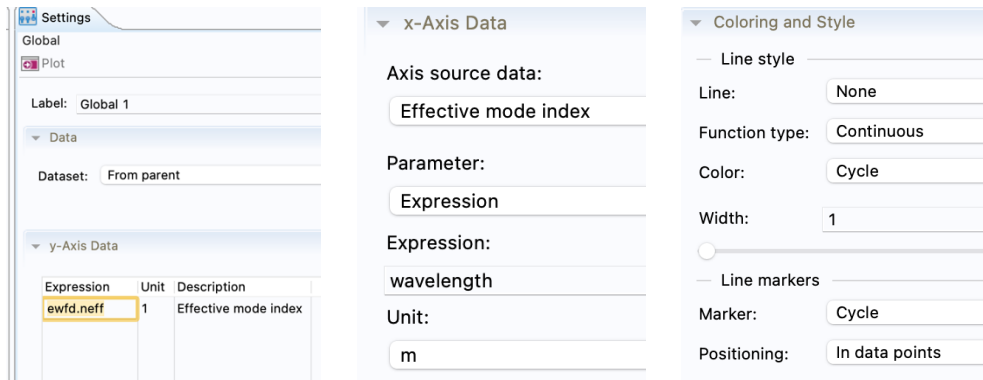
- Click "Plot". It plots all six n_{eff} values against wavelength. The data points are not connected with lines; otherwise, one can't distinguish the dispersion curves.
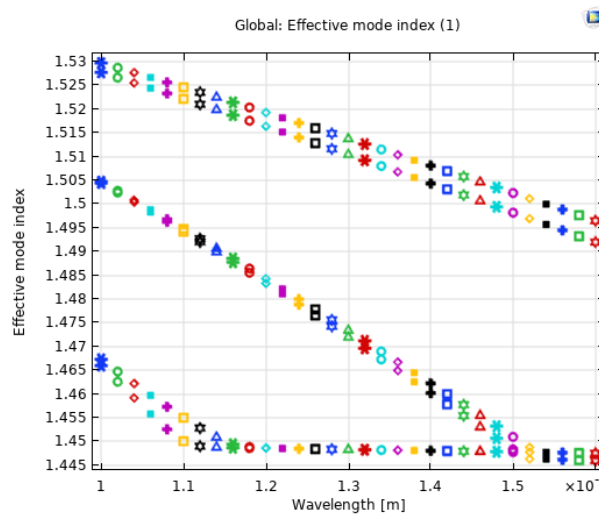
The top two dispersion curves correspond to the two fundamental modes, one with horizontal polarization and the other with vertical polarization. The middle group of dispersion curves correspond to second-order modes, and so on. Keep in mind that silica has refractive index 1.45. Modes with n_{eff} equal or close to 1.45 has their fields distributed predominately in silica region; therefore, they are not well guided. From the plot, cut-off wavelength of the waveguide is roughly identified as $\lambda_{cutoff} = 1.5 \, \mu m$.