Simulation of Metal–Air Surface Plasmon Polariton Propagation and Dispersion

Introduction

Electromagnetic waves that are confined to propagate along a surface, such as surface plasmon polaritons (SPPs), are of great research interest due to their potential applications in nanoscale manipulation of light. This model will discuss how to set up a simulation to visualize the propagation as well as the frequency versus propagation constant dispersion relationship of SPPs.

Propagating electromagnetic waves can exist in a variety of forms — such as plane waves, spherical waves, Gaussian beams, and so on. There are also propagating electromagnetic waves that are confined in space, such as waveguide modes propagating in metallic or dielectric waveguides.

In addition, there is another special type of electromagnetic wave that is confined to a planar surface. This type of wave propagates tangentially to the surface with exponentially decaying fields in the perpendicular direction. Its wavelength is often smaller than the free space wavelength at the same frequency. Thus, this type of wave provides promises for nanoscale control and manipulation of photons, which is desirable in many applications, ranging from optical communication and information processing to solar energy harvesting and digital displays.

The existence of this wave type was found at metal–dielectric interfaces and is known as surface plasmon polariton. The term plasmon refers to the collective oscillation of charges in a metal, whereas the term polariton generally refers to a quasi-particle that is the result of the coupling between a photon with a polar excitation in a material. The SPPs are the result of coupling of surface plasmons and light.

Model Definition

This model demonstrates SPPs in the simplest system that supports it, namely the bulk metal–dielectric interface. Imagine that the metal–dielectric interface is represented by the

xz plane at $y = 0$. The dielectric region is above the plane, $y > 0$, and the metal region is below the plane, $y < 0$. The surface wave propagates in the x direction.

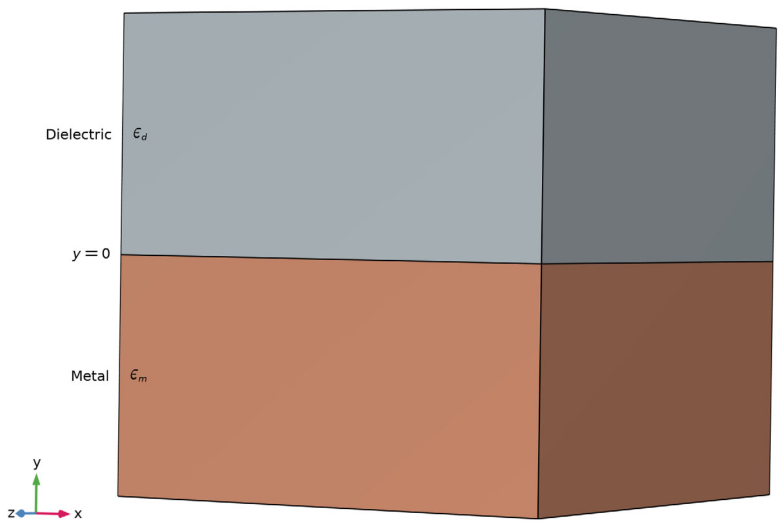


Figure 1: A metal–dielectric interface at $y = 0$. In this model, the SPP propagates in the x direction and exponentially decays in the y direction.

Here, it is of interest to study a TM mode surface wave. The expressions for the electric and magnetic fields in the dielectric and the metal are then given by

$$\mathbf{H}^d = (0,0,H_z^d)\exp(-j\beta x)\exp(-\gamma^d y) \tag{1}$$

$$\mathbf{E}^d = (E_x^d,E_y^d,0)\exp(-j\beta x)\exp(-\gamma^d y) \tag{2}$$

$$\mathbf{H}^m = (0,0,H_z^m)\exp(-j\beta x)\exp(\gamma^m y) \tag{3}$$

$$\mathbf{E}^m = (E_x^m,E_y^m,0)\exp(-j\beta x)\exp(\gamma^m y) \tag{4}$$

where the d and m superscripts denote quantities in dielectric and metallic domains, respectively. β is the complex SPP propagation constant. Both γ^d and γ^m are positive real numbers that describe the decay of the field away from the metal–dielectric interface.

The tangential components of the electric and magnetic fields, and the normal component of the electric displacement field, are continuous across the metal–dielectric boundary. Therefore,

$$E_x^d = E_x^m = E_x \tag{5}$$

$$H_z^d = H_z^m = H_z \tag{6}$$

$$\varepsilon_d E_y^d = \varepsilon_m E_y^m = D_y\,. \tag{7}$$

Since there is no external charge and the permittivity is constant inside the respective metallic and dielectric domains, $\nabla \cdot \mathbf{E} = 0$ must hold inside the two regions. Combining this condition with Equation 2 and Equation 4, gives the following two equations

$$-j\beta E_x = \gamma^d \frac{D_y}{\varepsilon_d} \tag{8}$$

$$-j\beta E_x = -\gamma^m \frac{D_y}{\varepsilon_m}\,. \tag{9}$$

Subsequently, if those two equations are combined, you get the simple relation

$$\frac{\gamma^d}{\varepsilon_d} = -\frac{\gamma^m}{\varepsilon_m}\,. \tag{10}$$

From this relation, it is clear why SPPs only exist between a dielectric, having a positive real part of the permittivity, and a metal, having a negative real part of the permittivity. To have the field decay in the y direction, both γ^d and γ^m must be positive, which means that the permittivities ε_d and ε_m must have opposite signs.

To derive the expression for the propagation constant β, the Helmholtz equation is used

$$\nabla^2 \mathbf{E} + k_0^2 \varepsilon \mu \mathbf{E} = 0\,, \tag{11}$$

where $k_0 = \omega / c$ is the free space wave number.Plugging Equation 2 and Equation 4 into the Helmholtz equation leads to

$$\beta^2 = \varepsilon_d k_0^2 - (\gamma^d)^2 \tag{12}$$

$$\beta^2 = \varepsilon_m k_0^2 - (\gamma^m)^2\,. \tag{13}$$

Finally, combining Equation 10, Equation 12, and Equation 13, the following expression for the SPP propagation constant is derived

$$\beta = \sqrt{\frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}} k_0 . \tag{14}$$

The real part of β is related to the SPP wavelength by $\lambda_{\mathrm{SPP}} = 2\pi/\mathrm{Re}(\beta)$, while the imaginary part describes the SPP propagation loss. Generally, the permittivities ε_d and ε_m are frequency dependent, so β is also frequency-dependent. The relationship between β and the frequency is often what needs to be known to characterize the SPPs in a system.

Remember that the above discussion is purely based on the assumption that the SPP is a TM wave. For the possibility of the TE wave, one can simply follow the previous derivation steps and show that all the field amplitudes must be zero. This means that SPPs only exist as a TM wave.

This model simulates SPPs propagating at the interface between silver (metal) and air (dielectric), using material properties for silver from the built-in Optical Material Library. Numeric ports are used on the left and right boundaries of the model. The left port, with excitation turned on, will launch the SPP, while the right port, with excitation turned off, will absorb the SPP without reflection. To get the mode field for both ports, two Boundary Mode Analysis study steps are added. Finally, a Frequency Domain study step is used when solving for the domain field.

Results and Discussion

Figure 2 shows the wave as it propagates in the *x* direction. The decay in the *y* direction is faster on the metal side due to the strong absorption.

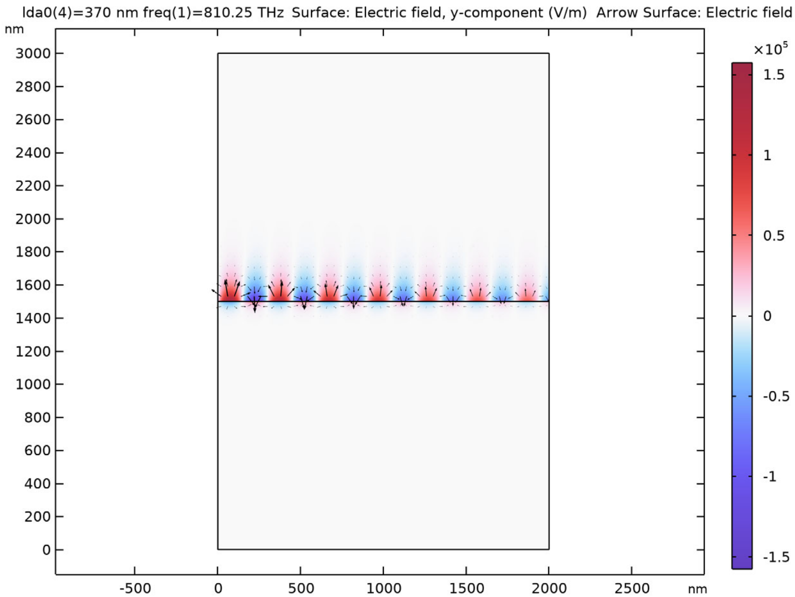


Figure 2: The y-component of the electric field for a wavelength of 370 nm (3.35 eV). The wave gets weaker, due to absorption, as it propagates from left to right. The arrows indicate the electric field strength and direction.

Figure 3 confirms that there is strong absorption for short wavelengths, whereas for longer wavelengths the transmission increases.

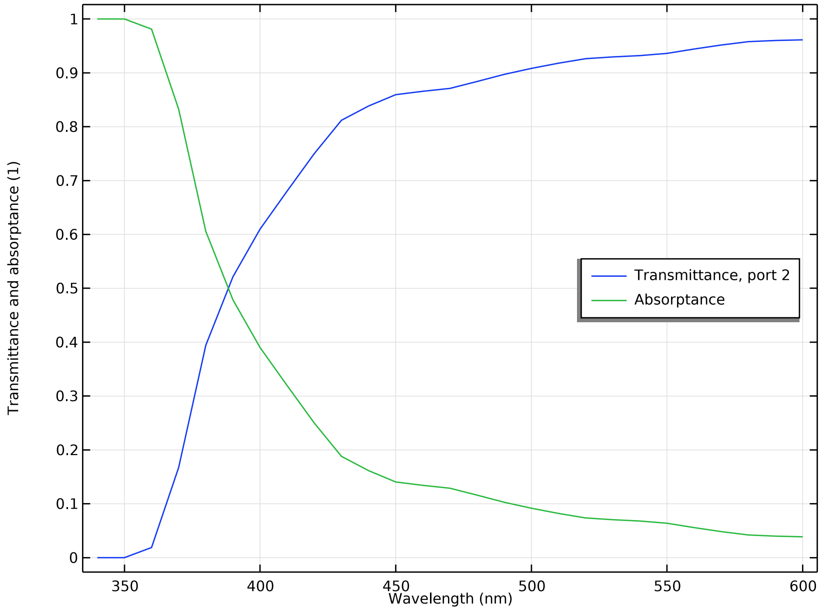


Figure 3: A plot of the transmittance and absorptance versus wavelength.

The mode field plot in Figure 4 clearly shows that the SPP decays much faster in the silver domain than in the air domain.

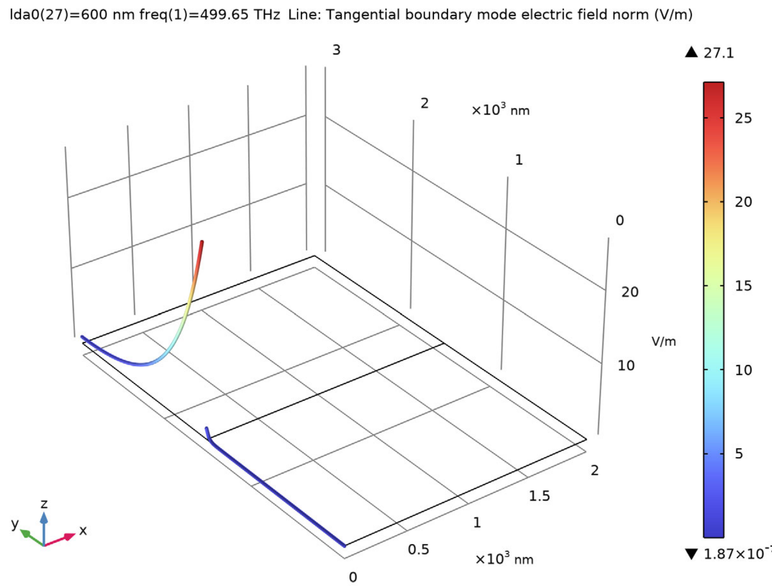


Figure 4: The norm of the electric mode field for Port 1.

To capture the quantitative relationship between the frequency (photon energy) and β, a plot of `freq*h_const` on the y-axis versus the propagation constant `ewfd.beta_1` on the x-axis (shown by the circle markers) is shown in Figure 5.

When studying SPPs, it is customary to define a figure of merit, often referred to as the Q factor, as the ratio of the real and the imaginary part of β. When β has a smaller imaginary part (equivalently, a larger Q factor), the SPP can propagate a long distance relative to its wavelength before it is attenuated. A larger Q factor is usually desirable for practical applications. The Q factor can conveniently be plotted using a color expression added to the dispersion curve. Here, a brighter color represents higher Q factors and a darker color represents lower Q factors. In addition, a dashed line representing $f = c/\lambda$, often called the light line, is added. The light line is the dispersion relation of free space photons. Lastly, the analytical expression from Equation 13 is plotted as a solid curve. The simulated dispersion and the analytical expression show good agreement.

The dispersion plot in Figure 5 is very representative for the SPP dispersion in noble metals. This plot is useful for gaining insight of the characteristics of SPPs. More importantly, it shows that the dispersion curve of SPPs always lies on the right side of the light line. The implication of this is that the SPP wavelength is always smaller than the wavelength of free space waves. This is why SPPs can be used as a way to compress the wavelength of light to achieve a higher field concentration.

Furthermore, the mismatch between the free-space wave number and the SPP propagation constant means that it is not possible to excite SPPs simply by shining light onto the metal surface. Some external mechanism to achieve phase matching is required. The excitation of SPPs is often done using total internal reflection from a prism or using diffraction from a grating. The goal of with these techniques is to prepare the electromagnetic field, so that its propagation constant matches that of the SPP at the same frequency.

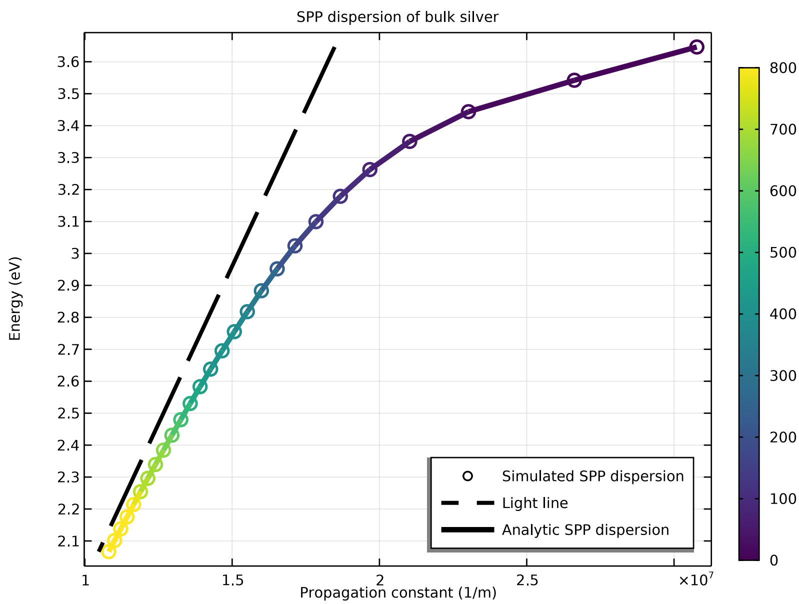


Figure 5: A plot of the simulated dispersion curve of the SPP at the interface between silver and air. The simulated result (circles) is consistent with the analytical calculation (solid line). The free space light dispersion, or light line, is represented by a dashed line. The color represents the Q factor of SPP.

For more SPP simulation examples, see the blog post in Ref. 1.

Reference

1. Xinzhong Chen, "Modeling Surface Plasmon Polaritons in COMSOL®," COMSOL Blog, 12 Oct. 2022; https://www.comsol.com/blogs/modeling-surface-plasmon-polaritons-in-comsol/.

Application Library path: `Wave_Optics_Module/Waveguides/metal_air_surface_plasmon_polariton`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Boundary Mode Analysis**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
L	2[um]	2E-6 m	Simulation domain length
H	3[um]	3E-6 m	Simulation domain height
lda0	400[nm]	4E-7 m	Wavelength
f0	c_const/lda0	7.4948E14 1/s	Frequency

The constant `c_const` above represents the speed of light.

GEOMETRY 1

The geometry is very simple, consisting of only one rectangle that is split into two halves.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
2. In the **Settings** window for **Geometry**, locate the **Units** section.
3. From the **Length unit** list, choose **nm**.

Rectangle 1 (r1)

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `L`.
4. In the **Height** text field, type `H`.
5. Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (nm)
`Layer 1`	`H/2`

6. Click **Build All Objects**.

MATERIALS

Pick silver from the Optical Material Library.

ADD MATERIAL

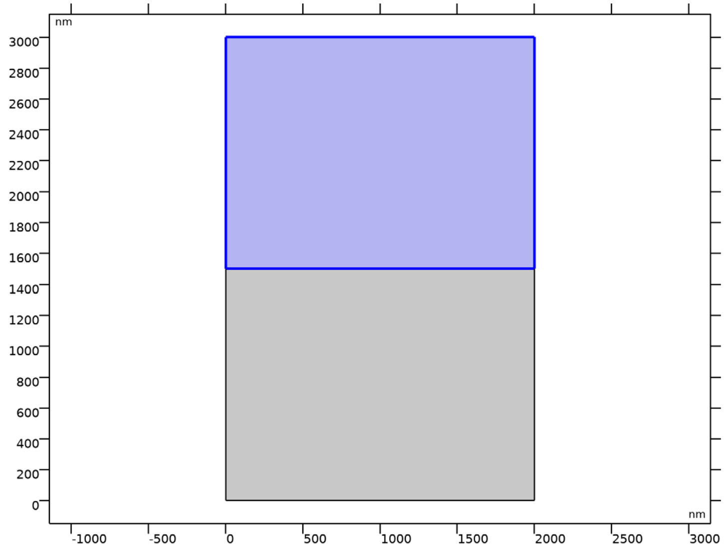
1. In the **Home** toolbar, click **Add Material** to open the **Add Material** window.
2. Go to the **Add Material** window.
3. In the tree, select **Optical>Inorganic Materials>Ag - Silver>Experimental data: bulk, thick film>Ag (Silver) (Johnson and Christy 1972: n,k 0.188-1.94 um)**.
4. Click **Add to Component** in the window toolbar.

MATERIALS

Air

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
2. In the **Settings** window for **Material**, type `Air` in the **Label** text field.

3 Select Domain 2 only.



4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Refractive index, real part	n_iso ; nii = n_iso, nij = 0	1	1	Refractive index

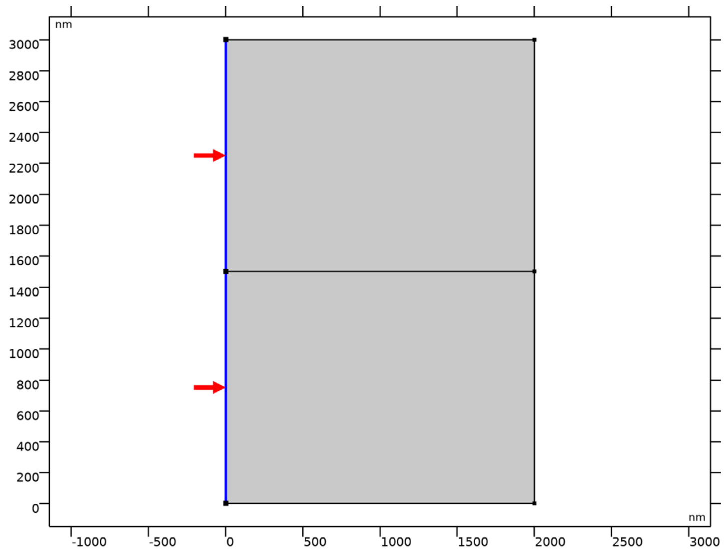
5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Port 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electromagnetic Waves, Frequency Domain (ewfd)** and choose **Port**.

2 Select Boundaries 1 and 3 only.



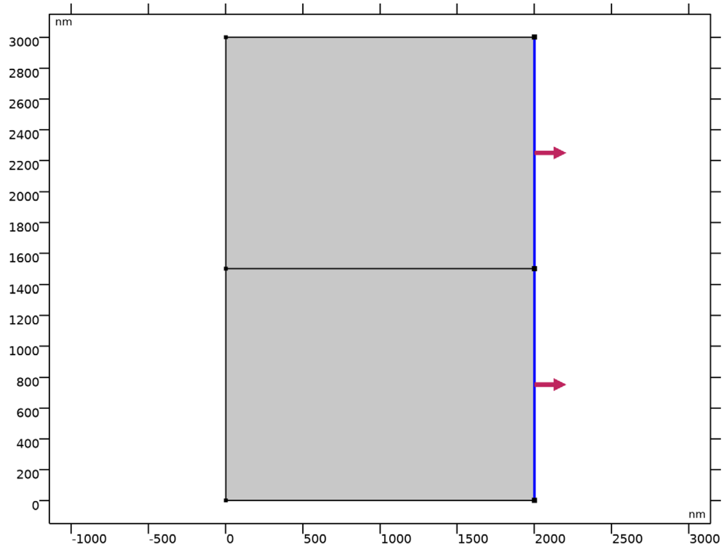
3 In the **Settings** window for **Port**, locate the **Port Properties** section.

4 From the **Type of port** list, choose **Numeric**.

Port 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Port**.

2 Select Boundaries 6 and 7 only.



3 In the **Settings** window for **Port**, locate the **Port Properties** section.

4 From the **Type of port** list, choose **Numeric**.

STUDY 1

Step 1: Boundary Mode Analysis

1 In the **Model Builder** window, under **Study 1** click **Step 1: Boundary Mode Analysis**.

2 In the **Settings** window for **Boundary Mode Analysis**, locate the **Study Settings** section.

3 In the **Mode analysis frequency** text field, type `f0`.

4 Select the **Search for modes around shift** check box. In the associated text field, type `5`.

5 Right-click **Study 1>Step 1: Boundary Mode Analysis** and choose **Duplicate**.

Step 3: Boundary Mode Analysis 1

1 In the **Model Builder** window, right-click **Step 3: Boundary Mode Analysis 1** and choose **Move Up**.

2 In the **Settings** window for **Boundary Mode Analysis**, locate the **Study Settings** section.

3 In the **Port name** text field, type `2`.

Step 3: Frequency Domain

1 In the **Model Builder** window, click **Step 3: Frequency Domain**.

2 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `f0`.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
lda0 (Wavelength)		nm

5 Click **Range**.

6 In the **Range** dialog box, type `340` in the **Start** text field.

7 In the **Step** text field, type `10`.

8 In the **Stop** text field, type `600`.

9 Click **Add**.

DEFINITIONS

Analytic 1 (an1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Local>Analytic**.

2 In the **Settings** window for **Analytic**, type `epsilonr` in the **Function name** text field.

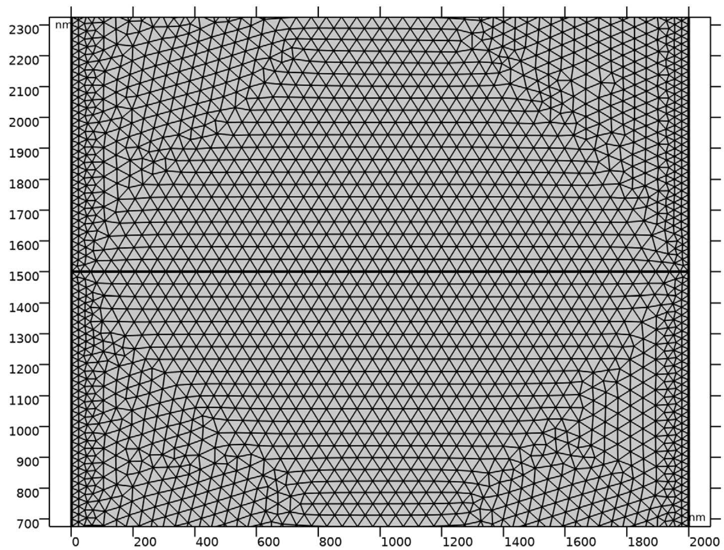
3 Locate the **Definition** section. In the **Expression** text field, type `(mat1.rfi.nr(x)-1i*mat1.rfi.ni(x))^2`.

4 Click to expand the **Advanced** section. Select the **May produce complex output for real arguments** check box.

This analytical function calculates the relative permittivity of silver.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.



2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size 2

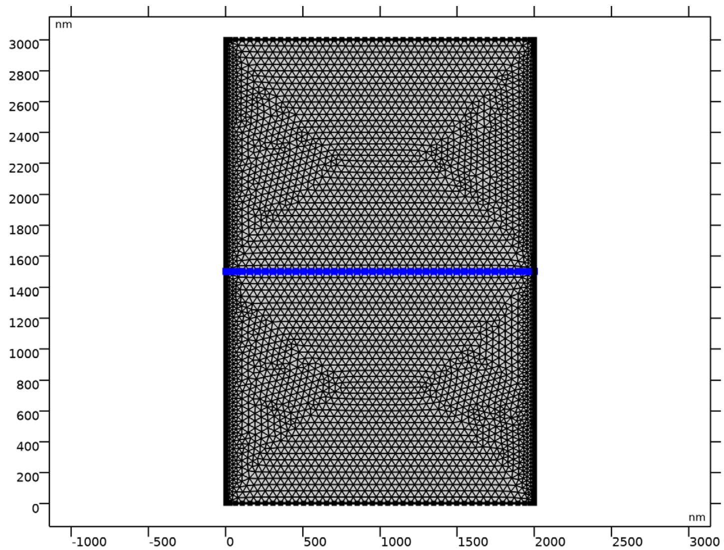
1 Right-click **Component 1 (comp1)>Mesh 1** and choose **Size**.

2 Drag and drop **Size 2** below **Size 1**.

3 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

4 From the **Geometric entity level** list, choose **Boundary**.

5 Select Boundary 4 only.



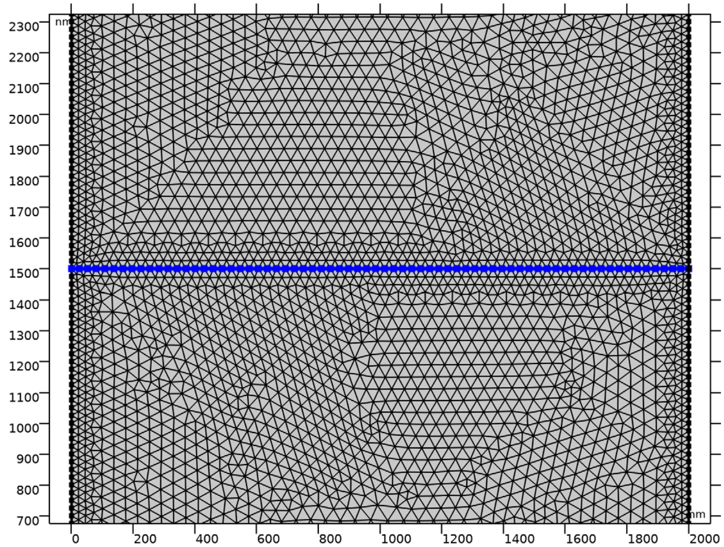
6 Locate the **Element Size** section. Click the **Custom** button.

7 Locate the **Element Size Parameters** section.

8 Select the **Maximum element size** check box. In the associated text field, type `(lda0/real(sqrt(epsilonr(lda0/1[m])/(1+epsilonr(lda0/1[m])))))/12`.

The maximum element size should be much smaller than SPP wavelength.

9 Click **Build All**.



The mesh at the metal-air interface is finer than the one built using Physics-controlled mesh.

STUDY 1

In the **Home** toolbar, click **Compute**.

RESULTS

Electric Field (ewfd)

1 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

2 From the **Parameter value (lda0 (nm))** list, choose **370**.

3 In the **Electric Field (ewfd)** toolbar, click **Plot**.

Surface 1

1 In the **Model Builder** window, expand the **Electric Field (ewfd)** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `ewfd.Ey`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Wave>WaveLight** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

8 From the **Scale** list, choose **Linear symmetric**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Electric Field (ewfd)** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Electromagnetic Waves, Frequency Domain>Electric>ewfd.Ex,ewfd.Ey - Electric field**.

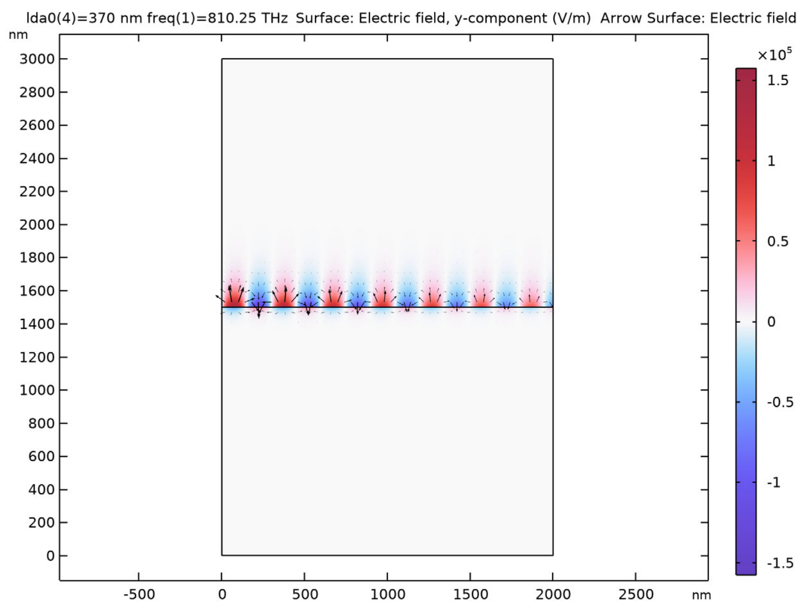
3 Locate the **Arrow Positioning** section. Find the **X grid points** subsection. In the **Points** text field, type `50`.

4 Find the **Y grid points** subsection. In the **Points** text field, type `50`.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

6 In the **Electric Field (ewfd)** toolbar, click **Plot**.

7 Select the **Scale factor** check box. In the associated text field, type `1e-3`.



Transmittance and Absorptance (ewfd)

Before creating the frequency versus propagation constant dispersion plot, it is good to inspect some of the default plots that are automatically generated when performing a simulation with Numeric ports.

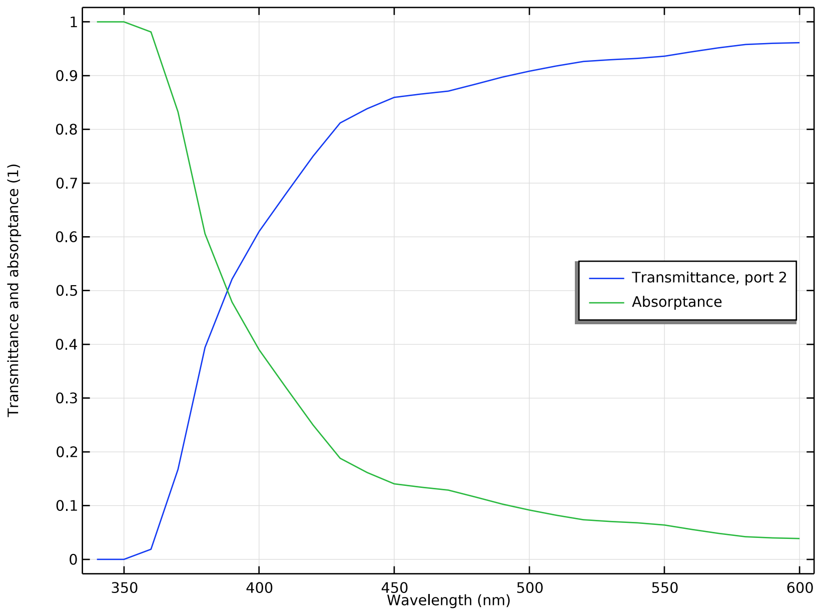
The reflectance is small and not of interest here. So, curves related to the reflectance will be removed from the plot.

1 In the **Model Builder** window, under **Results** click **Reflectance, Transmittance, and Absorptance (ewfd)**.
2 In the **Settings** window for **1D Plot Group**, type `Transmittance and Absorptance (ewfd)` in the **Label** text field.
3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Transmittance and absorptance (1)`.
4 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Global 1

1 In the **Model Builder** window, expand the **Transmittance and Absorptance (ewfd)** node, then click **Global 1**.
2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
3 Ctrl-click to select table rows 1 and 3.
4 Click **Delete**.

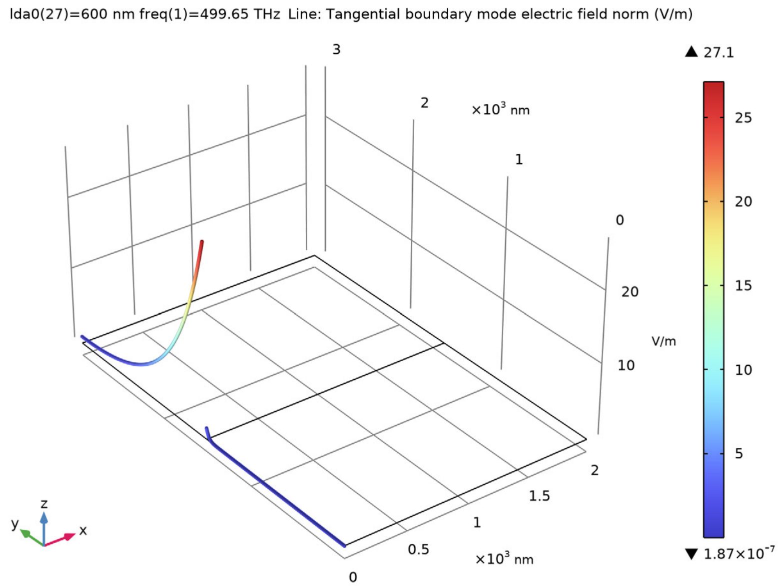
5 In the **Transmittance and Absorptance (ewfd)** toolbar, click **Plot**.



This figure shows that the absorption is large for short wavelengths and falls off to low values for longer wavelengths.

Electric Mode Field, Port 1 (ewfd)

1 In the **Model Builder** window, under **Results** click **Electric Mode Field, Port 1 (ewfd)**.



This figure shows the electric mode field norm for **Port 1**. It is clear that the wave decays rapidly in the metal and is extending more into the dielectric domain.

SPP Dispersion

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `SPP Dispersion` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol4)**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `SPP dispersion of bulk silver`.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Propagation constant (1/m)`.

8 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **SPP Dispersion** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`freq*h_const`	`eV`	`Energy`

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **All solutions**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `ewfd.beta_1`.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 From the **Width** list, choose **3**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

10 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

11 In the table, enter the following settings:

Legends
`Simulated SPP dispersion`

12 Right-click **Global 1** and choose **Duplicate**.

Global 2

1 In the **Model Builder** window, click **Global 2**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `ewfd.k0`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Black**.

6 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Light line`

Color Expression 1

1 In the **Model Builder** window, right-click **Global 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `-real(ewfd.beta_1)/imag(ewfd.beta_1)`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Linear>Viridis** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Color Expression**, click to expand the **Range** section.

8 Select the **Manual color range** check box.

9 In the **Minimum** text field, type `0`.

10 In the **Maximum** text field, type `800`.

Global 1

Right-click **Global 1** and choose **Duplicate**.

Global 3

1 In the **Model Builder** window, click **Global 3**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `ewfd.omega/c_const*sqrt(epsilonr(lda0)/(epsilonr(lda0)+1))`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

5 From the **Width** list, choose **4**.

6 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Analytic SPP dispersion`

Color Expression 1

1 In the **Model Builder** window, expand the **Global 3** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `real((ewfd.omega/c_const)*sqrt(epsilonr(lda0)/(epsilonr(lda0)+1)))/imag(-(ewfd.omega/c_const)*sqrt(epsilonr(lda0)/(epsilonr(lda0)+1)))`.

4 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

5 In the **SPP Dispersion** toolbar, click **Plot**.