Created in COMSOL Multiphysics 5.4

Scatterer on Substrate

Introduction

A plane TE-polarized electromagnetic wave is incident on a gold nanoparticle on a dielectric substrate. The absorption and scattering cross sections of the particle are computed for a few different polar and azimuthal angles of incidence.

Model Definition

Figure 1 shows the geometry, with the substrate considered to occupy the entire z<0 half-space. A plane electromagnetic wave, with a 500 nm wavelength, is incident at a polar angle θ and an azimuthal angle ϕ . The wave is plane-polarized with the electric field vector tangential to the surface of the substrate.

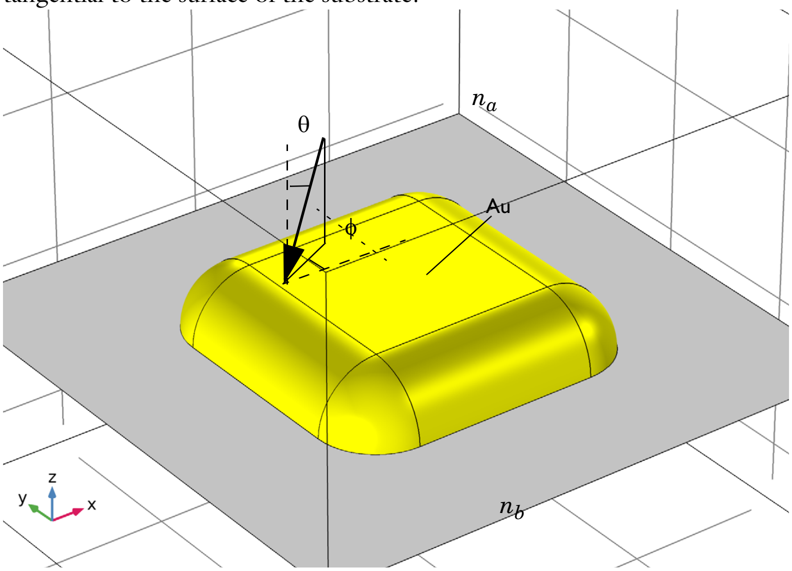


Figure 1: The modeled geometry. The gray boundary represents the surface of the dielectric. The electric field vector of the incident wave points in the ϕ direction, orthogonal to the plane of incidence.

The model uses $n_a = 1$ for air and $n_b = 1.5$ for the dielectric substrate. The scattering nanoparticle is made of gold. The refractive index is taken from the Optical Materials Database.

The model computes the scattering, absorption, and extinction cross-sections of the particle on the substrate. The scattering cross-section is defined as

$$\sigma_{sc} = \frac{1}{I_0}\iint(\mathbf{n} \cdot \mathbf{S}_{sc})dS$$

Here, $\mathbf{n}$ is the normal vector pointing outwards from the nanodot, $\mathbf{S}_{sc}$ is the scattered intensity (Poynting) vector, and I_0 is the incident intensity. The integral is taken over the closed surface of the scatterer. The absorption cross section equals

$$\sigma_{abs} = \frac{1}{I_0}\iiint Q dV$$

where Q is the power loss density in the particle and the integral is taken over its volume. The extinction cross section is simply the sum of the two others:

$$\sigma_{ext} = \sigma_{sc} + \sigma_{abs}$$

Results and Discussion

As explained in Notes About the COMSOL Implementation, the model first computes a background field from the plane wave incident on the substrate, and then uses that to arrive at the total field with the nanoparticle present.

Figure 2 and Figure 3 show the y-component and the norm of the electric background field, not yet affected by the nanoparticle, for the $\phi = \pi/4$, $\theta = \pi/6$ solution. In the air, this field is a superposition of the incident and reflected plane waves. In the substrate, only a transmitted plane wave exists.

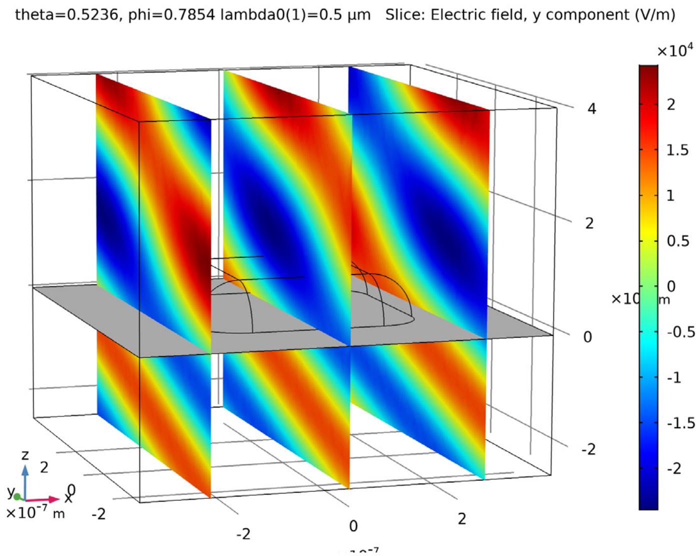


Figure 2: Background electric field, y-component for $\phi = \pi/4$*,* $\theta = \pi/6$*, on three slices parallel with the yz-plane.*

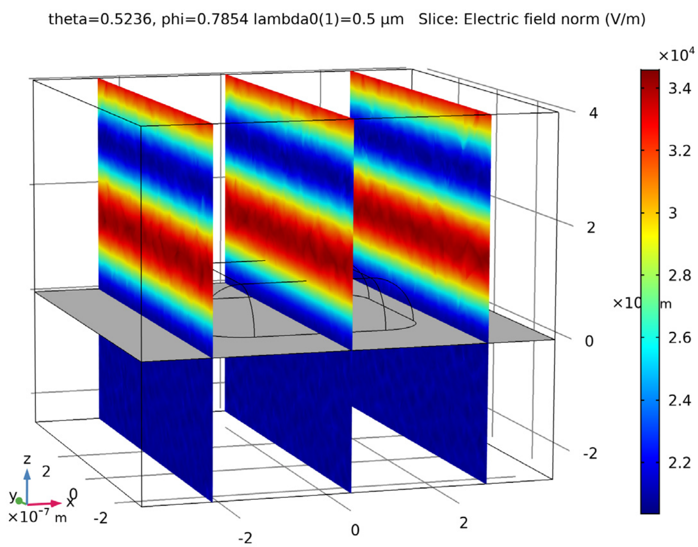


Figure 3: Background electric field norm, for $\phi = \pi/4$*,* $\theta = \pi/6$*.*

Figure 4 and Figure 5 show the norm of the total electric field for the same angles of incidence, after it has been influenced both by the material interface and by the nanoparticle.

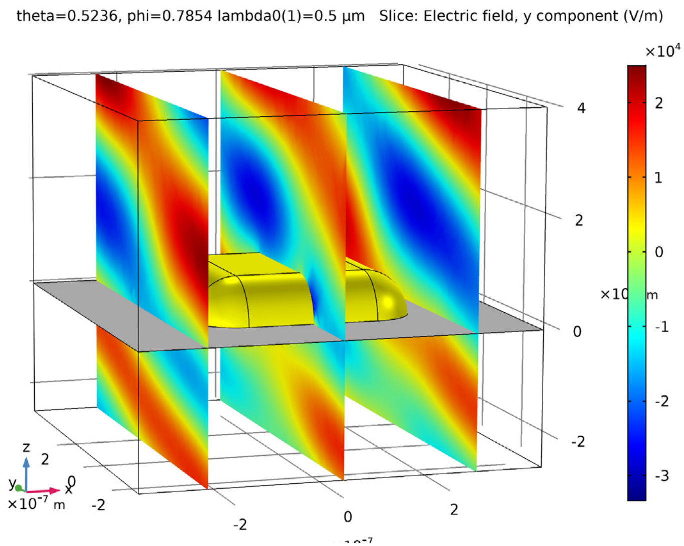


Figure 4: Slice plot of the y-component of the total electric field for $\phi = \pi/4$, $\theta = \pi/6$.

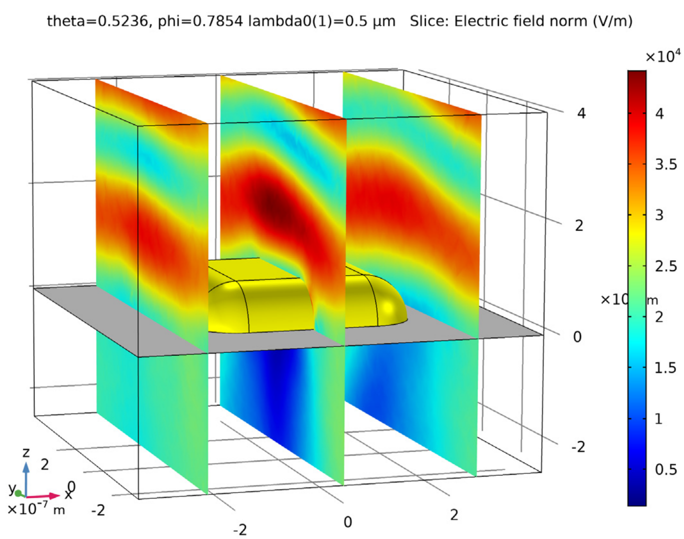


Figure 5: Slice plot of the total electric field norm for $\phi = \pi/4$, $\theta = \pi/6$.

In Figure 6, the power loss density is shown in a horizontal slice through the nanoparticle. No apparent resonance is present and most of the losses take place near the surface of the particle.

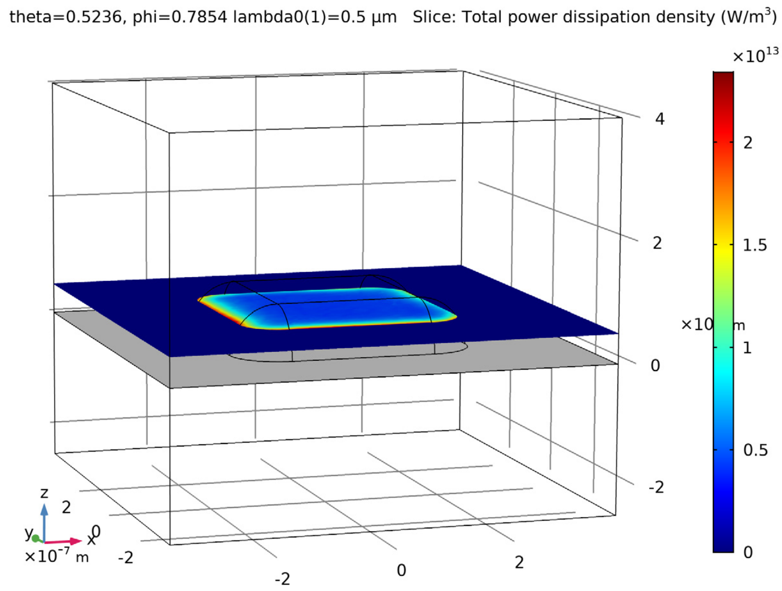


Figure 6: Power loss density in a slice through the nanoparticle.

Table 1 shows the computed cross sections for the set of angles of incidence.

TABLE 1: CROSS SECTIONS.

θ	ϕ	σ_{abs} **(m²)**	σ_{ext} **(m²)**
0	0	$9.45 \cdot 10^{-14}$	$2.28 \cdot 10^{-13}$
$\pi/6$	0	$8.10 \cdot 10^{-14}$	$1.95 \cdot 10^{-13}$
$\pi/6$	$\pi/4$	$8.14 \cdot 10^{-14}$	$1.97 \cdot 10^{-13}$
$\pi/4$	$\pi/4$	$6.67 \cdot 10^{-14}$	$1.58 \cdot 10^{-13}$

For this small sample of the angular space, both cross sections indicate a strong dependence on the polar angle but little variation with the azimuthal angle. For a comparison, the nanoparticle covers a geometric area of $1.59 \cdot 10^{-13}$ m^2 of the substrate.

Notes About the COMSOL Implementation

The Electromagnetic Waves, Frequency Domain interface features an option to solve for the scattered field, a perturbation to the total field caused by a local scatterer. The incident wave is then entered as a background electric field. This field should be a solution to the wave equation without the presence of the scatterer.

If the scatterer is suspended in free space or any other homogeneous medium, the background field is simply what you are sending in, for example a Gaussian or a plane wave. With the scatterer placed on a substrate, the analytical expression for the background field becomes more complicated. It needs to be the correct superposition of an incident and a reflected wave in the free space domain, and a transmitted wave in the substrate.

A simple and general way to avoid deriving and entering the analytical background field is to use a full field solution of the problem without the scatterer. To achieve this full field solution, the simulation is set up with two Port conditions. One defines the incident plane wave and allows for specular reflection. The other absorbs the transmitted plane wave. The side boundaries have Floquet conditions, stating that the solution on one side of the geometry equals the solution on the other side multiplied by a complex-valued phase factor. This effectively turns the model into a section of a geometry that extends indefinitely in the xy-plane.

The propagation direction and the polarization of the incident electric field are input parameters for the periodic ports. Internally, this information is also used by the Floquet conditions. Using the coordinate system in Figure 1, the incident wave vector is

$$\mathbf{k}_a = (k_x, k_y, k_{az}) = k_a(\cos\phi_a\sin\theta_a, \sin\phi_a\sin\theta_a, -\cos\theta_a)$$

where k_a is the wave number in the first medium, here vacuum, ϕ_a and θ_a the azimuthal and polar angles of incidence. The expression for the tangentially polarized electric field vector at the plane of incidence becomes

$$\mathbf{E}_0 = E_0(-\sin\phi_a, \cos\phi_a, 0)\exp(-i(k_x x + k_y y))$$

The Port condition lets you define a total input power from which the electric field amplitude E_0 is derived. The model uses the value

$$P = I_0 A\cos\theta$$

where $I_0 = 1\ \mathrm{MW/m^2}$ is the intensity of the incident field and A the area of the boundary where the port is set up.

In the substrate, the wave vector is

$$\mathbf{k}_b = (k_x, k_y, k_{bz}) = k_b(\cos\phi_b\sin\theta_b, \sin\phi_b\sin\theta_b, -\cos\theta_b)$$

with

$$k_b = \frac{n_b}{n_a}k_a$$

$$\phi_b = \phi_a$$

$$\sin\theta_b = \frac{n_a}{n_b}\sin\theta_a$$

Notice that the x and y components for the wave vector are the same for the wave in the substrate and the incident wave, due to field continuity.

The electric field vector at the output port is proportional to

$$(-\sin\phi_b, \cos\phi_b, 0)\exp(-i(k_x x + k_y y)) .$$

Thus, the mode fields and the mode field amplitudes are the same at the output port as at the input port.

Table 2 compares the results for the background field reflectance and the corresponding analytical value. For more information, see (Fresnel Equations).

TABLE 2: COMPUTED AND ANALYTICAL POWER REFLECTION COEFFICIENTS.

θ	ϕ	ewfd.Rport_1	R
0	0	0.0400	0.0400
π/6	0	0.0576	0.0578
π/6	π/4	0.0576	0.0578
π/4	π/4	0.0937	0.0920

A second Electromagnetic Waves, Frequency Domain interface introduces the gold nanoparticle as the scatterer and surrounds the geometry with PMLs. With the full field solution from the first interface as the background field, only the scattered field needs to be absorbed in the PMLs.

Application Library path: `Wave_Optics_Module/Optical_Scattering/scatterer_on_substrate`

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 **3D**.
2. In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.
3. Click **Add**.
4. In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.
5. Click **Add**.

   After clicking **Add** twice, you should now see two **Electromagnetic Waves, Frequency Domain** entries in the **Added physics interfaces** field.
6. Click **Study**.
7. In the **Select Study** tree, select **Empty Study**.

   You will add steps to the study before solving the model.
8. Click **Done**.

GLOBAL DEFINITIONS

Define the model parameters. The Description field is optional.

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**
w	750[nm]	7.5E-7 m	Width of physical geometry
t_pml	150[nm]	1.5E-7 m	PML thickness
h_air	400[nm]	4E-7 m	Air domain height
h_subs	250[nm]	2.5E-7 m	Substrate domain height
na	1	1	Refractive index, air
nb	1.5	1.5	Refractive index, substrate
lda0	500[nm]	5E-7 m	Wavelength
phi	0	0	Azimuthal angle of incidence in both media
theta	0	0	Polar angle of incidence in air
thetab	asin(na/nb* sin(theta))	0 rad	Polar angle in substrate
I0	1[MW/m^2]	1E6 W/m²	Intensity of incident field
P	I0*w^2*cos(theta)	5.625E-7 W	Port power

The first four parameters will be used in defining the geometry. The azimuthal angle in the substrate remains the same as the angle of incidence. As the polar angle of incidence gets other values in the study, the polar angle in the substrate will automatically be recomputed.

GEOMETRY 1

Import the nanoparticle.

Import 1 (imp1)

1 In the **Home** toolbar, click **Import**.

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

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `scatterer_on_substrate.mphbin`.

5 Click **Import**.

Block 1 (blk1)

Draw the air and the substrate using your model parameters.

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w+2*t_pml`.

4 In the **Depth** text field, type `w+2*t_pml`.

5 In the **Height** text field, type `h_air+t_pml`.

6 Locate the **Position** section. From the **Base** list, choose **Center**.

7 In the **z** text field, type `(h_air+t_pml)/2`.

8 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	t_pml

9 Select the Left, Right, Front, Back, and Top check boxes.

10 Clear the Bottom check box.

Block 2 (blk2)

1 Right-click **Block 1 (blk1)** and choose **Duplicate**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Height** text field, type `h_subs+t_pml`.

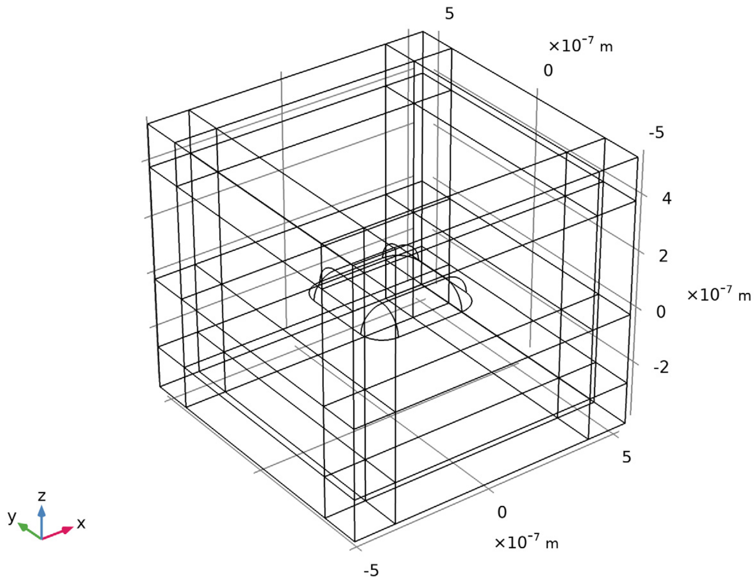
4 Locate the **Position** section. In the **z** text field, type `-(h_subs+t_pml)/2`.

5 Make sure the Left, Right, Front, Back, and Bottom check boxes are selected. Leave the Top check box cleared.

6 Click **Build All Objects**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

8 Click the **Wireframe Rendering** button in the **Graphics** toolbar.



DEFINITIONS

Define selections to separate between the part of your model where you will compute physical results and the part that will constitute the PML. For convenience, add separate selections for the nanoparticle.

Explicit 1

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Physical Domains` in the **Label** text field.

3 Select Domains 18, 19, and 25 only.

Complement 1

1 In the **Definitions** toolbar, click **Complement**.

2 In the **Settings** window for **Complement**, type `PML Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to invert**, click **Add**.

4 In the **Add** dialog box, select **Physical Domains** in the **Selections to invert** list.

5 Click **OK**.

Explicit 2

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Nanoparticle` in the **Label** text field.

3 Select Domain 25 only.

Explicit 3

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Nanoparticle Surface` in the **Label** text field.

3 Select Domain 25 only.

4 Locate the **Output Entities** section. From the **Output entities** list, choose **Adjacent boundaries**.

Perfectly Matched Layer 1 (pml1)

1 In the **Definitions** toolbar, click **Perfectly Matched Layer**.

2 In the **Settings** window for **Perfectly Matched Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **PML Domains**.

4 Locate the **Scaling** section. From the **Physics** list, choose **Electromagnetic Waves, Frequency Domain 2 (ewfd2)**.

Variables 1

Only the second interface will be active in the PML domains. As this interface will use the electric field components from the first interface, define them to be `0` in the PML domains.

1 In the **Definitions** toolbar, click **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **PML Domains**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
ewfd.Ex	0		
ewfd.Ey	0		
ewfd.Ez	0		

MATERIALS

Define materials for the air, the substrate, and the nanoparticle.

Material 1 (mat1)

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 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	na	1	Refractive index

Material 2 (mat2)

1 Right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, type `Substrate` in the **Label** text field.

3 Select Domains 1, 2, 5, 6, 9, 10, 13, 14, 17, 18, 21, 22, 26, 27, 30, 31, 34, and 35 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	nb	1	Refractive index

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

Add the material properties of gold from the Optical Materials Database.

2 Go to the **Add Material** window.

3 In the tree, select **Optical>Inorganic Materials>Au - Gold>Models and simulations>Au (Gold) (RakiÄá et al. 1998: Brendel-Bormann model; n,k 0.248-6.20 µm)**.

4 Click **Add to Component** in the window toolbar.

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

MATERIALS

Au (Gold) (RakiÄá et al. 1998: Brendel-Bormann model; n,k 0.248-6.20 µm) (mat3)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Nanoparticle**.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

You are now ready to specify the physics. Start by setting up the first interface so that it computes the full wave solution to the plane wave falling in on the semi-infinite substrate.

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

2 In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Physical Domains**.

4 Locate the **Physics-Controlled Mesh** section. Clear the **Enable** check box, as the mesh will be setup manually in some later steps.

Wave Equation, Electric 2

1 In the **Physics** toolbar, click **Domains** and choose **Wave Equation, Electric**.

2 In the **Settings** window for **Wave Equation, Electric**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Nanoparticle**.

4 Locate the **Electric Displacement Field** section. From the n list, choose **User defined**. In the associated text field, type `na`.

5 From the k list, choose **User defined**. This redefines the nanoparticle as air.

DEFINITIONS

Define variables for the mode field amplitudes to the ports, as the expressions are entered twice (on both ports).

Variables 2

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

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

4 Select Boundaries 62 and 68 only.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
E0x	-sin(phi)		
E0y	cos(phi)		

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Port 1

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

2 Select Boundary 68 only.

For the first port, wave excitation is **on** by default.

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

4 In the P_{in} text field, type `P`.

5 From the **Type of port** list, choose **Periodic**, as the background field is an infinite plane-wave field.

Now use the variables, defined for the mode field amplitudes.

6 Locate the **Port Mode Settings** section. Specify the $\mathbf{E}_0$ vector as

E0x	x
E0y	y
0	z

Finally, add the angles of incidence and the refractive index for the domain adjcacent to the port.

7 In the α_1 text field, type `theta`.

8 In the α_2 text field, type `phi`.

9 Locate the **Automatic Diffraction Order Calculation** section. In the n text field, type `na`.

Port 2

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

2 Select Boundary 62 only.

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

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

Again, use the variables defined for the mode field amplitudes.

5 Locate the **Port Mode Settings** section. Specify the $\mathbf{E}_0$ vector as

E0x	x
E0y	y
0	z

6 Locate the **Automatic Diffraction Order Calculation** section. In the n text field, type `nb`.

Periodic Condition 1

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

2 Select Boundaries 60, 63, 113, and 116 only.

3 In the **Settings** window for **Periodic Condition**, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet periodicity**.

5 From the **k-vector for Floquet periodicity** list, choose **From periodic port**.

Periodic Condition 2

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

2 Select Boundaries 61, 64, 74, and 77 only.

3 In the **Settings** window for **Periodic Condition**, locate the **Periodicity Settings** section.

4 From the **Type of periodicity** list, choose **Floquet periodicity**.

5 From the **k-vector for Floquet periodicity** list, choose **From periodic port**.

ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN 2 (EWFD2)

Set up the second interface to compute how the plane wave solution from the first interface is affected by the nanoparticle.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain 2 (ewfd2)**.

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

3 From the **Formulation** list, choose **Scattered field**.

4 Specify the $\mathbf{E}_\mathrm{b}$ vector as

ewfd.Ex	x
ewfd.Ey	y
ewfd.Ez	z

5 Locate the **Physics-Controlled Mesh** section. Clear the **Enable** check box, as the mesh will be setup manually in some later steps.

MESH 1

Define a mesh with a maximum mesh element size of one sixth of the material wavelength. In the nanoparticle, the mesh should resolve the 43 nm skin depth. To avoid interpolation errors across the periodic boundaries, they should be meshed identically. PMLs should preferably use a swept mesh with at least six elements across.

Start by adding a **Size** node and a **Free Tetrahedral** node.

Size

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

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `lda0/6`, which will be the maximum mesh element size for the Air domain.

Now add a **Size** node for the nanoparticle.

Size 1

1. In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.
2. Right-click **Size 1** and choose **Move Up**.
3. In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
4. From the **Geometric entity level** list, choose **Domain**.
5. Select Domain 25 only.
6. Locate the **Element Size** section. Click the **Custom** button.
7. Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.
8. In the associated text field, type `43[nm]`.

Create the **Size** node for the substrate domain by duplicating this size node.

Size 2

1. Right-click **Component 1 (comp1)>Mesh 1>Size 1** and choose **Duplicate**.
2. In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
3. Click **Clear Selection**.
4. Select Domain 18 only.
5. Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `lda0/6/nb`.

Add a triangular mesh for two of the periodic boundary condition boundaries and then use **Copy Mesh** to make the mesh boundaries identical.

Free Triangular 1

1. In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Free Triangular**.
2. Select Boundaries 60, 61, 63, and 64 only.

Copy Face 1

1. Right-click **Mesh 1** and choose **More Operations>Copy Face**.
2. Select Boundaries 60 and 63 only.
3. In the **Settings** window for **Copy Face**, locate the **Destination Boundaries** section.
4. Select the **Active** toggle button.
5. Select Boundaries 113 and 116 only.

Copy Face 2

1 Right-click **Component 1 (comp1)>Mesh 1>Copy Face 1** and choose **Duplicate**.

2 In the **Settings** window for **Copy Face**, locate the **Source Boundaries** section.

3 Click **Clear Selection**.

4 Select Boundaries 61 and 64 only.

5 Locate the **Destination Boundaries** section. Click **Clear Selection**.

6 Select Boundaries 74 and 77 only.

Free Tetrahedral 1

Before creating the final swept mesh, define the domains for the free tetrahedral mesh.

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Free Tetrahedral 1**.

2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domains 18, 19, and 25 only.

Swept 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.

2 Right-click **Swept 1** and choose **Move Down**.

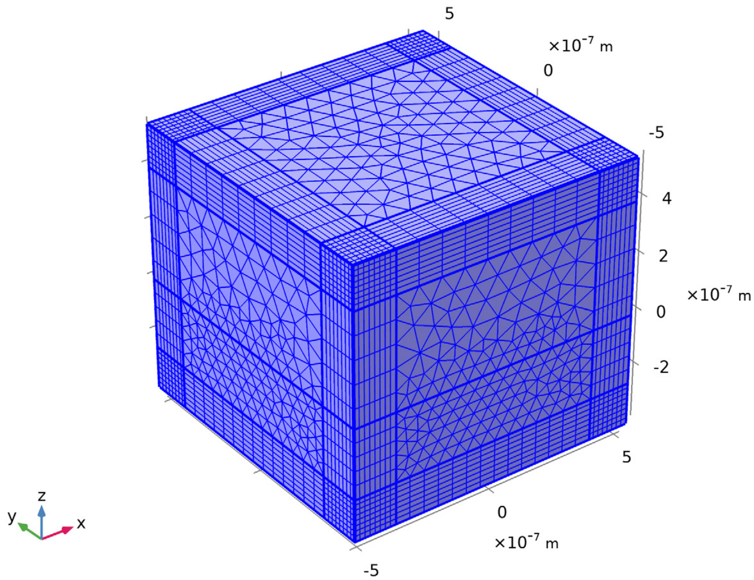
Distribution 1

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

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

3 In the **Number of elements** text field, type 8.

4 Click **Build All**.



DEFINITIONS

Before solving the model, set up component couplings and variables for extracting the cross sections.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `intop_vol` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **Nanoparticle**.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `intop_surf` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Nanoparticle Surface**.

Variables 3

1 In the **Definitions** toolbar, click **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
nrelPoav	nx*ewfd2.relPoavx+ny*ewfd2.relPoavy+nz*ewfd2.relPoavz	W/m²	Relative normal Poynting flux
sigma_sc	intop_surf(nrelPoav)/I0	m²	Scattering cross section
sigma_abs	intop_vol(ewfd2.Qh)/I0	m²	Absorption cross section
sigma_ext	sigma_sc+sigma_abs	m²	Extinction cross section

The relative normal Poynting vector is defined from the outwards-facing normal vector and the automatically defined coordinate components of the Poynting flux.

STUDY 1

Set up the solver for a few different combinations of angles. Because the second physics interface depends on the first one but not vice versa, the model can be solved sequentially.

1 In the **Model Builder** window, click **Study 1**.

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

3 Clear the **Generate default plots** check box.

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
theta (Polar angle of incidence in air)	0 pi/6 pi/6 pi/4	

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
phi (Azimuthal angle of incidence in both media)	0 0 pi/4 pi/4	

Step 1: Wavelength Domain

1 In the **Study** toolbar, click **Study Steps** and choose **Frequency Domain> Wavelength Domain**.
2 In the **Settings** window for **Wavelength Domain**, locate the **Study Settings** section.
3 In the **Wavelengths** text field, type `lda0`.
4 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for the **Electromagnetic Waves, Frequency Domain 2 (ewfd2)** interface.

Step 2: Wavelength Domain 2

1 In the **Study** toolbar, click **Study Steps** and choose **Frequency Domain> Wavelength Domain**.
2 In the **Settings** window for **Wavelength Domain**, locate the **Study Settings** section.
3 In the **Wavelengths** text field, type `lda0`.
4 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for the **Electromagnetic Waves, Frequency Domain (ewfd)** interface.
5 In the **Study** toolbar, click **Compute**.

RESULTS

Before generating the plots, set up the data sets for easy display of the surfaces of the substrate and the nanoparticle.

In the **Model Builder** window, expand the **Results** node.

Study 1/Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Results>Data Sets** node, then click **Study 1/ Solution 1 (sol1)**.
2 In the **Settings** window for **Solution**, type `Substrate` in the **Label** text field.
3 Right-click **Results>Data Sets>Substrate** and choose **Selection**.

Selection

1 In the **Model Builder** window, under **Results>Data Sets>Substrate (sol1)** click **Selection**.
2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.
3 From the **Geometric entity level** list, choose **Boundary**.
4 Select Boundaries 65 and 87 only.

Substrate 1 (sol1)

1 In the **Model Builder** window, under **Results>Data Sets** right-click **Substrate (sol1)** and choose **Duplicate**.

2 In the **Settings** window for **Solution**, type `Particle` in the **Label** text field.

Selection

1 In the **Model Builder** window, expand the **Results>Data Sets>Particle (sol1)** node, then click **Selection**.

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

3 From the **Selection** list, choose **Nanoparticle Surface**.

Study 1/Parametric Solutions 1 (sol2)

In the **Model Builder** window, under **Results>Data Sets** right-click **Study 1/ Parametric Solutions 1 (sol2)** and choose **Selection**.

Selection

1 In the **Model Builder** window, under **Results>Data Sets>Study 1/ Parametric Solutions 1 (sol2)** click **Selection**.

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

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Physical Domains**.

5 Select the **Propagate to lower dimensions** check box.

The selection you just made will make the fields show up only in the physical domain. If you want to see how the relative field is damped in the PML, you can delete this selection.

3D Plot Group 1

You will create plots for the *y* component and the norm of the background field and the total field. Begin with a plot of the background field, with the substrate but not the nanoparticle in place.

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Background Field, y` in the **Label** text field.

3 Locate the **Data** section. From the **Data set** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

Slice 1

1 Right-click **Background Field, y** and choose **Slice**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain>Electric>Electric field - V/m>ewfd.Ey - Electric field, y component**.

3 Locate the **Plane Data** section. In the **Planes** text field, type `3`.

4 In the **Background Field, y** toolbar, click **Plot**. You have now plotted the *y* component from the first interface, for the $\theta = \phi = \pi/4$ solution. You can look at the different solutions using the **Parameter Value** list.

Background Field, y

1 In the **Model Builder** window, under **Results** click **Background Field, y**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Parameter value (theta,phi)** list, choose **3: theta=0.5236, phi=0.7854**.

4 In the **Background Field, y** toolbar, click **Plot**.

Color only the substrate surface to make it clear that you are looking at the field distribution without the nanoparticle.

Surface 1

1 Right-click **Results>Background Field, y** and choose **Surface**.

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

3 From the **Data set** list, choose **Substrate (sol1)**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

5 Click to expand the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

7 From the **Color** list, choose **Gray**. If you zoom in and rotate the plot you just created, it should look like Figure 2.

Background Field, y

The most convenient way to reproduce Figure 3 is to duplicate and modify the *y* component plot.

Background Field, y 1

1 Right-click **Background Field, y** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Background Field, Norm` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Results>Background Field, Norm** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain>Electric>ewfd.normE - Electric field norm - V/m**.

3 In the **Background Field, Norm** toolbar, click **Plot**. The electric field norm from the first interface confirms that you have a standing wave pattern in the air and a propagating plane wave in the substrate.

Derived Values

In order to further confirm that the first interface was set up correctly, verify that the power reflection at the material interface agrees with the analytical result.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

Expression	Unit	Description
`ewfd.Rport_1`	`1`	`Reflectance, port 1`

5 Click **Evaluate**. The results agree reasonably well with the analytical solution, as indicated in Table 2.

Background Field, y

To visualize the total field, start out with another copy of one of your background field plots. You will change the plot expression and add the particle.

Background Field, y 1

1 In the **Model Builder** window, under **Results** right-click **Background Field, y** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Total Field, y` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Results>Total Field, y** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain 2>Electric>Electric field - V/m>ewfd2.Ey - Electric field, y component**.

Surface 2

1 In the **Model Builder** window, under **Results** right-click **Total Field, y** and choose **Surface**.

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

3 From the **Data set** list, choose **Particle (sol1)**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

7 From the **Color** list, choose **Yellow**. The plot should now look like Figure 4.

Total Field, y

Create a plot of the total field norm to reproduce Figure 5.

Total Field, y 1

1 Right-click **Total Field, y** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Total Field, Norm` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Results>Total Field, Norm** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain 2>Electric>ewfd2.normE - Electric field norm - V/m**.

3 In the **Total Field, Norm** toolbar, click **Plot**.

Derived Values

The cross section expressions that you defined are available for global evaluation.

Global Evaluation 2

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Data set** list, choose **Study 1/Parametric Solutions 1 (sol2)**.

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

Expression	Unit	Description
`sigma_abs`	`m^2`	`Absorption cross section`

5 Click **Evaluate**.

6 In the table, enter the following settings:

Expression	Unit	Description
`sigma_sc`	`m^2`	`Scattering cross section`

7 Click **Evaluate**.

8 In the table, enter the following settings:

Expression	**Unit**	**Description**
`sigma_ext`	`m^2`	`Extinction cross section`

9 Click **Evaluate**. The results should resemble those in Table 1.

Total Field, Norm

The remaining instructions result in a plot of the power loss in the particle, reproducing Figure 6.

Total Field, Norm 1

1 In the **Model Builder** window, under **Results** right-click **Total Field, Norm** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Power Loss` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Results>Power Loss** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1>Electromagnetic Waves, Frequency Domain 2>Heating and losses>ewfd2.Qh - Total power dissipation density - W/m³**.

3 Locate the **Plane Data** section. From the **Plane** list, choose **XY-planes**.

4 From the **Entry method** list, choose **Coordinates**.

5 In the **Z-coordinates** text field, type `50[nm]`.

Surface 2

In the **Model Builder** window, under **Results>Power Loss** right-click **Surface 2** and choose **Disable**.