Optical Scattering off a Gold Nanosphere

Introduction

This model demonstrates the calculation of the scattering of a plane wave of light off a gold nanosphere. The scattering is computed for the optical frequency range, over which gold can be modeled as a material with negative complex-valued permittivity. The far-field pattern and the losses are computed.

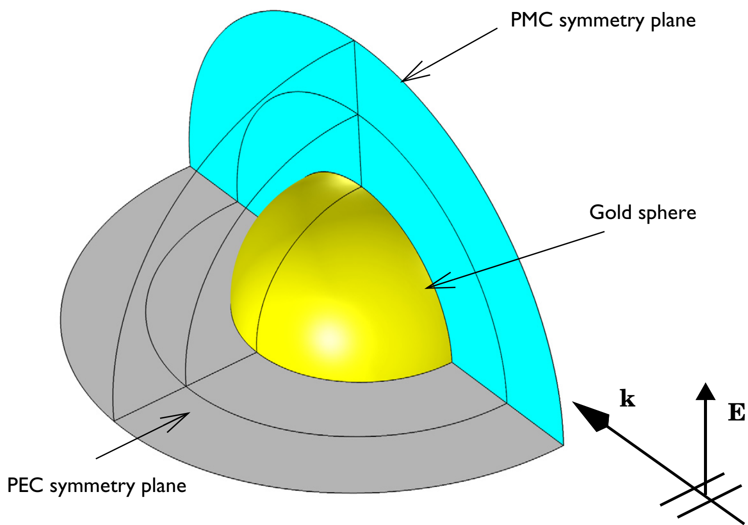


Figure 1: A gold sphere illuminated by a plane wave. Due to symmetry, only one-quarter of the sphere has to be modeled.

Model Definition

A gold sphere of radius r = 100 nm is illuminated by a plane wave, as shown in Figure 1. The free space wavelength range from 400 nm to 700 nm is simulated. The complex refractive index of gold is taken from the Optical Material Library, where interpolation functions for a large number of commonly used optical materials are found. Figure 2 shows the real and the imaginary parts of the refractive index for gold, for the wavelength range used in the simulation.

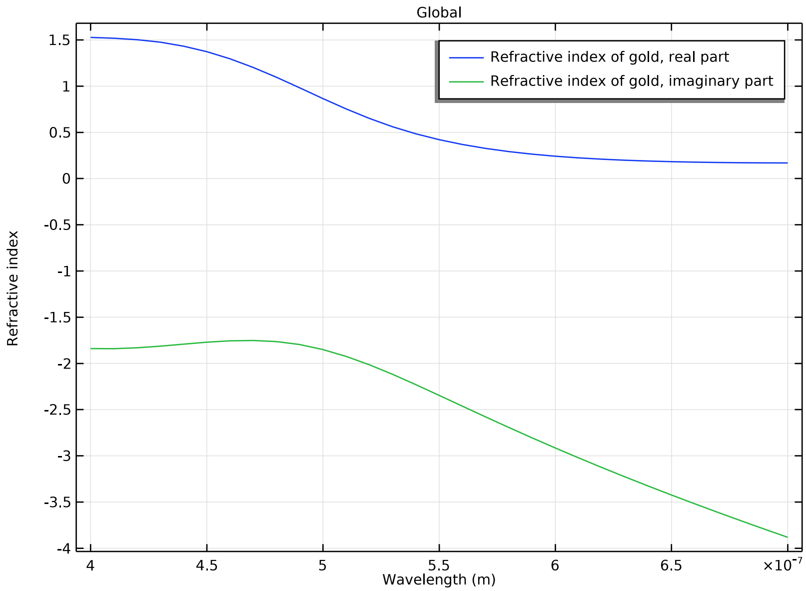


Figure 2: The real and the imaginary parts of the refractive index for gold.

From the refractive index, the relative permittivity is found from the relation

$$\varepsilon_r = \varepsilon' - j\varepsilon'' = (n' - jn'')^2,$$

where the real parts of the relative permittivity and the refractive index are denoted with primes and, similarly, the imaginary parts are denoted with bis. Figure 3 shows the relative permittivity, corresponding to the refractive index plotted in Figure 2. Notice that the real part of the relative permittivity is negative for this wavelength range.

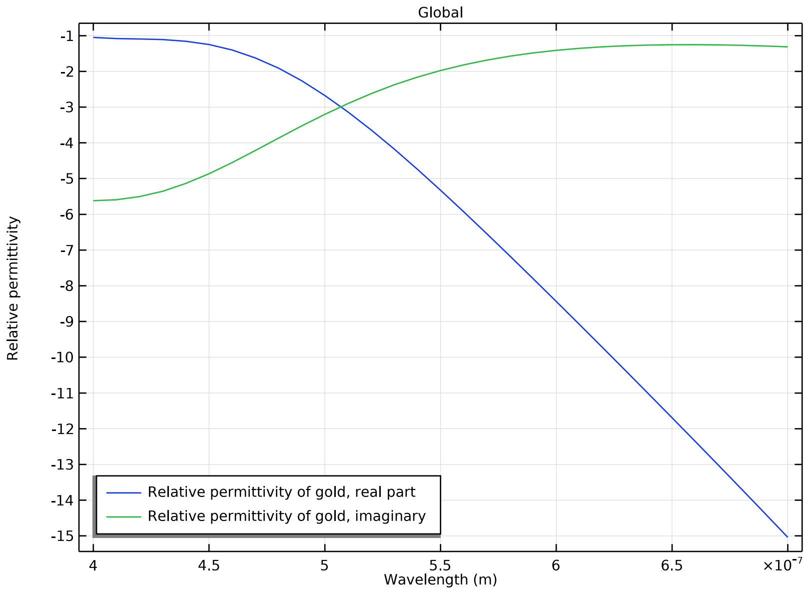


Figure 3: The real and the imaginary parts of the relative permittivity of gold.

Over the wavelength range of interest, it is possible to compute the skin depth via

$$\delta = \frac{1}{Re\sqrt{-k_0^2\varepsilon_r}}$$

where k_0 is the free space wave number, and ε_r is the complex-valued relative permittivity. The skin depth is shown in Figure 4, and ranges from 28 nm to 44 nm. The skin depth is evaluated with assumption of plane wave incidence over flat surface, so it is not directly applicable on the gold sphere in the model.

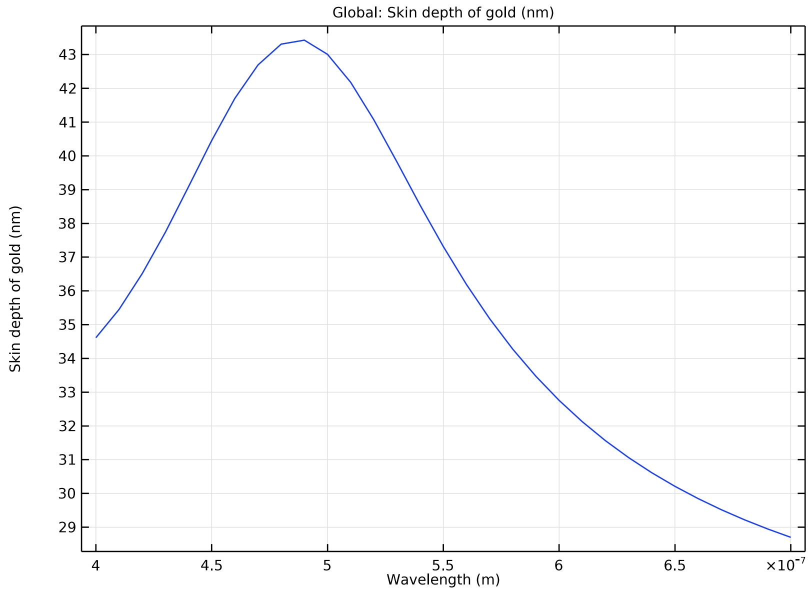


Figure 4: The skin depth of gold.

Due to the symmetry of the problem, only one-quarter of the sphere is modeled. A region of air around the sphere is also modeled, of width equal to half the wavelength in free space. A perfectly matched layer (PML) domain is outside of the air domain and acts as an absorber of the scattered field. The PML should not be within the reactive near-field of the scatterer, placing it a half-wavelength away is usually sufficient. The far-field radiation pattern and the heat losses are computed.

Results and Discussion

The far-field patterns show that, at short wavelengths, a single gold sphere scatters light forward, in the direction of propagation of the incident light. At longer wavelengths, the scattered fields from the sphere look more as the radiation pattern of a dipole antenna. The far-field radiation pattern for a wavelength of 700 nm is plotted in Figure 5. The E-plane and H-plane notation originates from antenna theory, where the E-plane denotes the plane containing the electric field polarization and the direction of maximum radiation, whereas the H-plane denotes the plane containing the magnetic field and the direction of maximum radiation. In this case, the E-plane denotes the *xz*-plane and the H-plane denotes the *xy*-plane.

The heat losses, plotted in Figure 6, show that the particle preferentially absorbs the shorter wavelengths. The radius of the sphere can also be varied to see how the absorption depends upon the geometry.

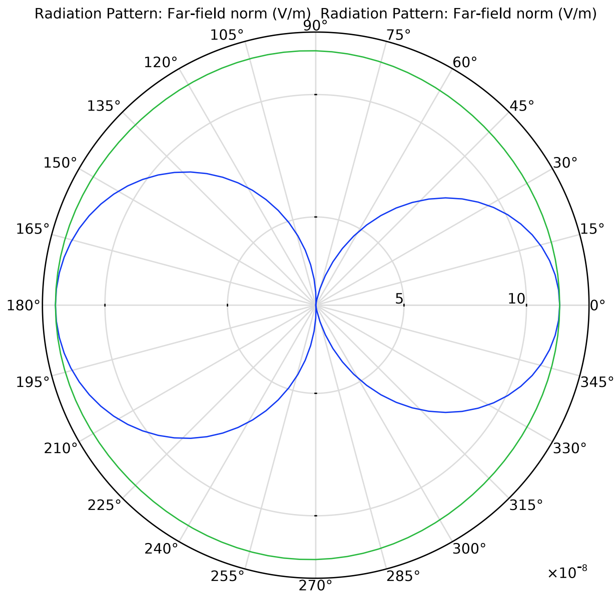


Figure 5: The far-field radiation pattern in the E-plane (blue) and H-plane (green) when wavelength is 700 nm.

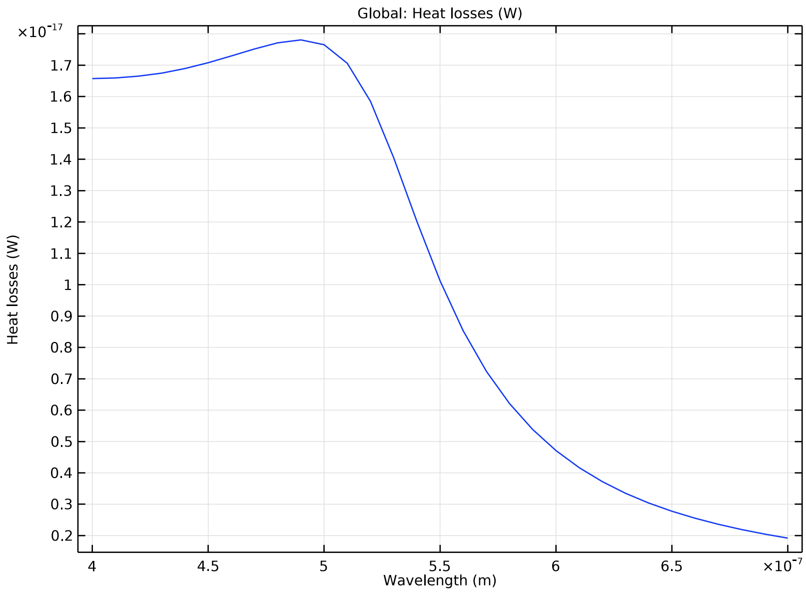


Figure 6: The resistive heating losses in the gold sphere.

Application Library path: `Wave_Optics_Module/Optical_Scattering/scattering_nanosphere`

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 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Wavelength Domain**.

6 Click **Done**.

GLOBAL DEFINITIONS

Define some parameters that are useful for setting up the geometry and the study.

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
r0	100[nm]	1E-7 m	Sphere radius
lda	400[nm]	4E-7 m	Wavelength
t_air	lda/2	2E-7 m	Thickness of air around sphere
t_pml	lda/2	2E-7 m	Thickness of PML

Here, c_const is a predefined COMSOL constant for the speed of light.

GEOMETRY 1

Create a sphere with layers. The outermost layer represents the PMLs and the core represents the gold sphere. The middle layer is the air domain.

Sphere 1 (sph1)

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

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

3 In the **Radius** text field, type r0+t_air+t_pml.

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

Layer name	Thickness (m)
Layer 1	t_pml
Layer 2	t_air

5 Click **Build Selected**.

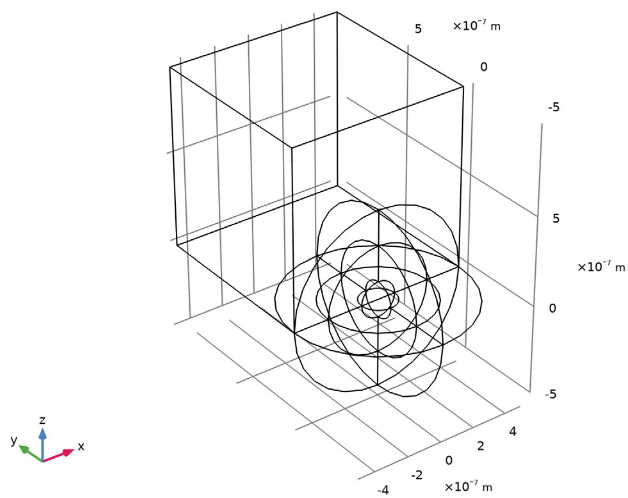
Choose wireframe rendering to get a better view of the interior parts.

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

Block 1 (blk1)

Then, add a block intersecting one-quarter of the sphere.

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 `2*(r0+t_air+t_pml)`.
4 In the **Depth** text field, type `2*(r0+t_air+t_pml)`.
5 In the **Height** text field, type `2*(r0+t_air+t_pml)`.
6 Locate the **Position** section. In the **x** text field, type `-(r0+t_air+t_pml)`.
7 Click **Build Selected**.
8 In the **Model Builder** window, click **Geometry 1**.

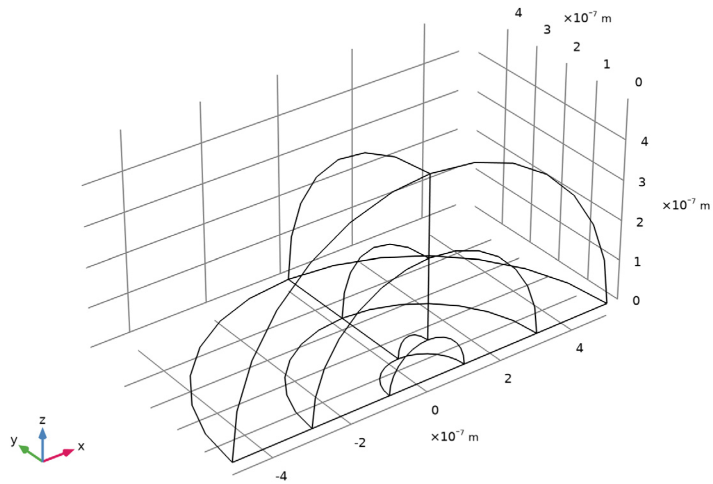


Intersection 1 (int1)

Generate the quarter sphere by intersecting two objects.

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Intersection**.
2 Click in the **Graphics** window and then press Ctrl+A to select both objects.
3 In the **Settings** window for **Intersection**, click **Build All Objects**.

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



DEFINITIONS

Add a variable for the total heat losses in the gold sphere computed as a volume integral of resistive losses. First, add a nonlocal integration coupling for the volume integral of the gold sphere.

Integration 1 (intop1)

1. In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.
2. In the **Settings** window for **Integration**, type `int_L` in the **Operator name** text field.
3. Select Domain 3 only.

Variables 1

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

   Add the heat loss variable for gold and variables representing the refractive index, the relative permittivity, and the skin depth of gold.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
l_gold	int_L(ewfd.Qrh)	W	Heat losses
n_gold	int_L(ewfd.nxx-j* ewfd.kixx)/(pi*r0^3/3)		Refractive index of gold
epsilonr_gold	n_gold^2		Relative permittivity of gold
deltaS_gold	1/real(sqrt(-(ewfd.k0* n_gold)^2))	m	Skin depth of gold

Here, the `ewfd.` prefix gives the correct physics-interface scope for the resistive losses. By calculating the average refractive index for the gold sphere, this averaged variable can later be evaluated in a global plot.

MATERIALS

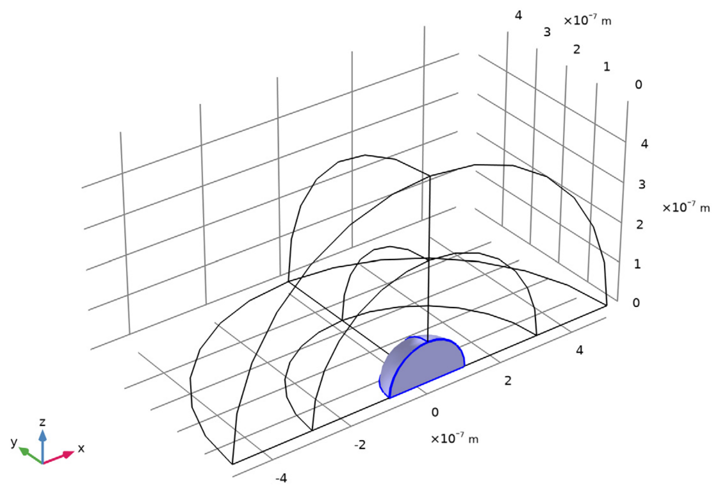
Assign air as the material for all domains, except for the gold sphere.

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 **Built-in>Air**.
4. Click **Add to Component** in the window toolbar.
5. In the tree, select **Optical>Inorganic Materials>Au - Gold>Models and simulations> Au (Gold) (Rakic et al. 1998: Brendel-Bormann model; n,k 0.248-6.20 um)**.
6. Click **Add to Component** in the window toolbar.
7. In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Au (Gold) (Rakic et al. 1998: Brendel-Bormann model; n,k 0.248-6.20 um) (mat2)
Select Domain 3 only.



ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Now set up the physics. You solve the model for the scattered field, so it needs background electric field (E-field) information. The background plane wave is traveling in the positive x direction, with the electric field polarized along the z-axis. The default boundary condition is perfect electric conductor, which applies to all exterior boundaries including the boundaries perpendicular to the background E-field polarization.

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 **Formulation** section.

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

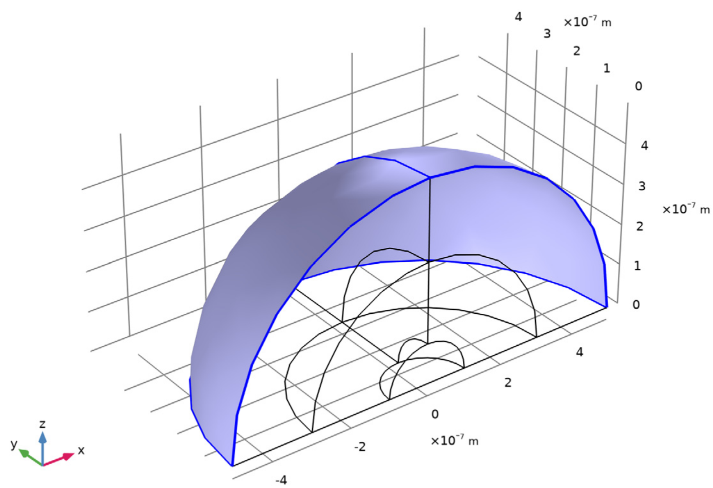
4 Specify the $\mathbf{E}_b$ vector as

0	x
0	y
exp(-j*ewfd.k0*x)	z

Scattering Boundary Condition 1

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

2 Select Boundaries 3 and 16 only.



DEFINITIONS

The outermost domains from the center of the sphere are the PMLs.

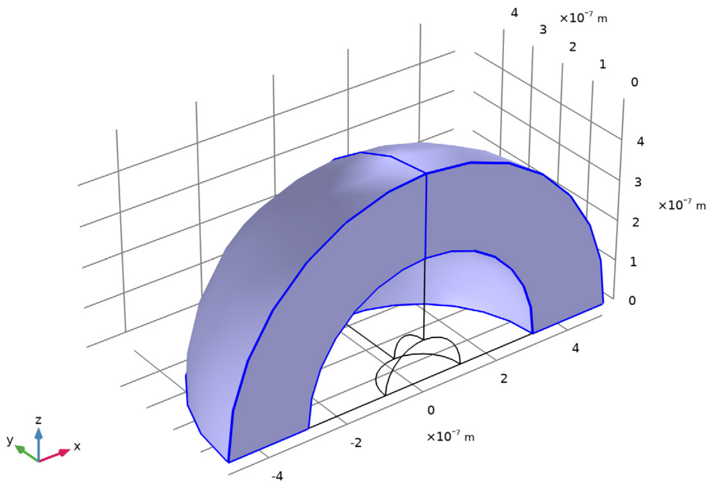
Perfectly Matched Layer 1 (pml1)

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

2 Select Domains 1 and 5 only.

3 In the **Settings** window for **Perfectly Matched Layer**, locate the **Geometry** section.

4 From the **Type** list, choose **Spherical**.



ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

Set PEC symmetry plane on the boundaries normal to the background E-field and PMC symmetry plane on the boundaries parallel to the background E-field polarization.

Symmetry Plane, PEC

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

2 In the **Settings** window for **Symmetry Plane**, type `Symmetry Plane, PEC` in the **Label** text field.

3 Select Boundaries 2, 5, 9, 17, and 18 only.

4 Locate the **Symmetry Plane** section. From the **Symmetry type** list, choose **Zero tangential electric field (PEC)**.

Symmetry Plane, PMC

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

2 In the **Settings** window for **Symmetry Plane**, type `Symmetry Plane, PMC` in the **Label** text field.

3 Select Boundaries 1, 4, 8, 11, and 14 only.

Far-Field Domain 1

In the **Physics** toolbar, click **Domains** and choose **Far-Field Domain**.

Far-Field Calculation 1

1 In the **Model Builder** window, expand the **Far-Field Domain 1** node, then click **Far-Field Calculation 1**.

2 In the **Settings** window for **Far-Field Calculation**, locate the **Far-Field Calculation** section.

3 From the **Symmetry settings** list, choose **From symmetry plane(s)**.

MESH 1

Automatically define the mesh from the specified wavelength and the material parameters.

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

2 In the **Settings** window for **Mesh**, locate the **Electromagnetic Waves, Frequency Domain (ewfd)** section.

3 From the **Maximum mesh element size control parameter** list, choose **Wavelength**.

4 In the **Minimum vacuum wavelength** text field, type `lda`.

5 Select the **Resolve wave in lossy media** check box, to resolve the field down to the skin depth in the gold sphere.

STUDY 1

Add a parametric sweep to create a new mesh for each wavelength in the sweep.

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
lda (Wavelength)	`range(400[nm],300[nm]/30,700[nm])`	`m`

Step 1: Wavelength Domain

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

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

3 In the **Wavelengths** text field, type `lda`.

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

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

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

7 In the **Study** toolbar, click **Compute**.

RESULTS

Begin the results analysis and visualization by adding a selection to see the resistive losses only inside the gold sphere.

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

Selection

1 In the **Model Builder** window, expand the **Results>Datasets** node.

2 Right-click **Study 1/Parametric Solutions 1 (sol2)** and choose **Selection**.

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

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

5 Select Domain 3 only.

3D Plot Group 1

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

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

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

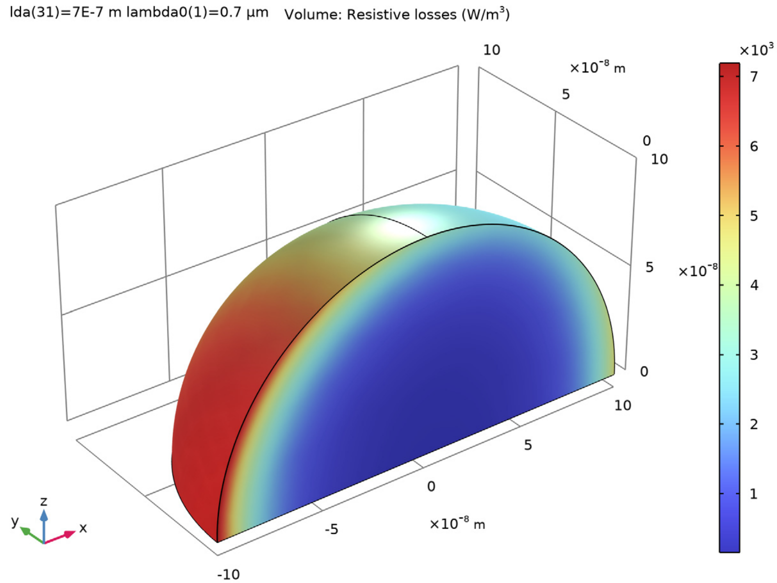
Volume 1

1 Right-click **3D Plot Group 1** and choose **Volume**.

2 In the **Settings** window for **Volume**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Electromagnetic Waves, Frequency Domain>Heating and losses>ewfd.Qrh - Resistive losses - W/m³**.

3 In the **3D Plot Group 1** toolbar, click **Plot**.

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



Polar Plot Group 2

The following instructions reproduce the polar plot of the far-field at the E-plane and H-plane shown in Figure 5.

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

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

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

4 From the **Parameter selection (lda)** list, choose **Last**.

Radiation Pattern 1

1 In the **Polar Plot Group 2** toolbar, click **More Plots** and choose **Radiation Pattern**.

2 In the **Settings** window for **Radiation Pattern**, locate the **Evaluation** section.

3 Find the **Angles** subsection. In the **Number of angles** text field, type 100.

4 Find the **Normal vector** subsection. In the **y** text field, type 1.

5 In the **z** text field, type 0.

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

7 In the table, enter the following settings:

Legends
`E-plane`

8 In the **Polar Plot Group 2** toolbar, click **Plot**.

The E-plane in this model is located on the *xz*-plane where angle ϕ is measured counterclockwise from the *x*-axis.

Polar Plot Group 2

Add the H-plane polar plot.

In the **Model Builder** window, click **Polar Plot Group 2**.

Radiation Pattern 2

1 In the **Polar Plot Group 2** toolbar, click **More Plots** and choose **Radiation Pattern**.

2 In the **Settings** window for **Radiation Pattern**, locate the **Evaluation** section.

3 Find the **Angles** subsection. In the **Number of angles** text field, type `100`.

4 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
`H-plane`

6 In the **Polar Plot Group 2** toolbar, click **Plot**.

1D Plot Group 3

The following instructions create a plot of the heat losses inside the gold sphere (see Figure 6).

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

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

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

Global 1

1 Right-click **1D Plot Group 3** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>l_gold - Heat losses - W**.

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

4 Click to expand the **Legends** section. Clear the **Show legends** check box.

1D Plot Group 3

1 In the **Model Builder** window, click **1D Plot Group 3**.

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

3 Select the **x-axis label** check box. In the associated text field, type `Wavelength (m)`.

4 In the **1D Plot Group 3** toolbar, click **Plot**. Compare the resulting plot with Figure 6.

1D Plot Group 4

Finally, add plots showing the real and the imaginary parts of the refractive index and the relative permittivity of gold, as well as the skin depth.

1 Right-click **Results>1D Plot Group 3** and choose **Duplicate**.

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

3 Select the **y-axis label** check box. In the associated text field, type `Refractive index`.

Global 1

1 In the **Model Builder** window, expand the **1D Plot Group 4** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>n_gold - Refractive index of gold - 1**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`real(n_gold)`	`1`	`Refractive index of gold, real part`
`imag(n_gold)`	`1`	`Refractive index of gold, imaginary part`

4 Locate the **Legends** section. Select the **Show legends** check box.

5 From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Refractive index of gold, real part`
`Refractive index of gold, imaginary part`

7 In the **1D Plot Group 4** toolbar, click **Plot**. Compare the resulting plot with Figure 2.

1D Plot Group 5

In the **Model Builder** window, under **Results** right-click **1D Plot Group 4** and choose **Duplicate**.

Global 1

1 In the **Model Builder** window, expand the **1D Plot Group 5** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>epsilonr_gold - Relative permittivity of gold - 1**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	**Unit**	**Description**
`real(epsilonr_gold)`	1	`Relative permittivity of gold, real part`
`imag(epsilonr_gold)`	1	`Relative permittivity of gold, imaginary part`

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

Legends
`Relative permittivity of gold, real part`
`Relative permittivity of gold, imaginary part`

1D Plot Group 5

1 In the **Model Builder** window, click **1D Plot Group 5**.

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

3 In the **y-axis label** text field, type `Relative permittivity`.

4 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

5 In the **1D Plot Group 5** toolbar, click **Plot**. Compare the resulting plot with Figure 3 and notice that the real part of the relative permittivity is negative in this wavelength range.

1D Plot Group 6

In the **Model Builder** window, under **Results** right-click **1D Plot Group 3** and choose **Duplicate**.

Global 1

1 In the **Model Builder** window, expand the **1D Plot Group 6** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>deltaS_gold - Skin depth of gold - m**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`deltaS_gold`	`nm`	`Skin depth of gold`

4 In the **1D Plot Group 6** toolbar, click **Plot**. Compare the resulting plot with Figure 4.