Rapid Thermal Annealing

Introduction

In the semiconductor industry, rapid thermal annealing (RTA) is a semiconductor process step used for the activation of dopants and the interfacial reaction of metal contacts. In principle, the operation involves rapid heating of a wafer from ambient to approximately 1000–1500 K. As soon as the wafer reaches this temperature, it is held there for a few seconds and then finally quenched. A rapid process step is crucial to avoid too much diffusion of the dopants. Furthermore, it is also important to avoid overheating and nonuniform temperature distributions to occur. An RTA apparatus, schematically shown in Figure 1, uses high-power IR lamps as heat sources (Ref. 1).

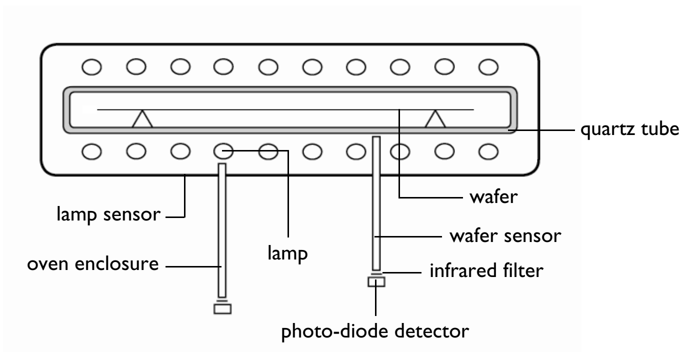


Figure 1: Diagram of a typical RTA (rapid thermal annealing) apparatus.

A technical difficulty lies in how to properly measure the wafer's temperature during the process. Two commonly used technical solutions are: thermocouples and IR sensors.

To achieve an accurate measurement, it is important that the temperature sensor is not subjected to direct radiation from the lamp. Ideally positioned, the sensor only receives secondary radiation; that is, the radiation reflected and emitted by the silicon wafer. Desirable characteristics of the sensor are high accuracy and short response time. While a high-performance design requires superior electronics, the sensor geometry plays a big role. In a nutshell, the sensor needs to be large enough to register a sufficient amount of radiation but light enough to minimize its own thermal inertia. Since COMSOL Multiphysics gives you control over the geometry, a parameter optimization of the sensor could be an exciting project. But first, justify that an infrared sensor is indeed more appropriate than the inexpensive thermocouple.

Model Definition

Figure 1 illustrates a typical RTA configuration. In many applications, RTA makes use of double-sided heating, in which IR lamps are positioned both above and below the silicon wafer. In this example we are modeling a single-sided heating apparatus, as shown in Figure 2.

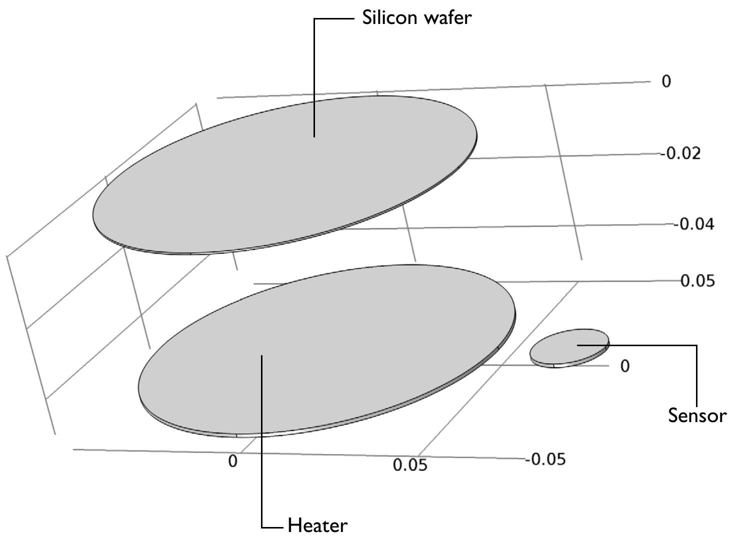


Figure 2: The model geometry.

The components in Figure 2 are contained in a chamber with temperature-controlled walls with a set point of 400 K. This results in a closed cavity so you can omit the geometry of the chamber walls. Furthermore, the model assumes that this physical system is dominated by radiation and convection cooling. The convective cooling of the wafer and sensor to the gas (at 400 K) is modeled using a heat transfer coefficient, h (in this example set to 20 $\mathrm{W/(m^2 \cdot K)}$).

The problem is governed by the heat equation, given below together with its boundary conditions:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q$$

$$-\mathbf{n} \cdot (-k\nabla T) = h(T_{\mathrm{inf}} - T) + \frac{\varepsilon}{1-\varepsilon}(J_0 - \sigma T^4)$$

Here ρ is the density; k denotes the thermal conductivity; Q represents the volume heat source; $\mathbf{n}$ is the surface normal vector; T_{inf} equals the temperature of the convection cooling gas; ε denotes the surface emissivity; J_0 is the expression for surface radiosity (further described in the *Heat Transfer Module User's Guide*); and σ is the Stefan-Boltzmann constant.

The model simulates the lamp as a solid object with a volume heat source of 25 kW. It is insulated on all surfaces except the top, which faces the silicon wafer. At this surface, heat leaves the lamp as radiation only. In order to capture the lamp's transient startup time, the model uses a low heat capacity, C_p, for the solid (10 J/(kg·K)). The lamp's other thermal properties are identical to those of copper metal (the default value in the interface).

In this case assume that the wafer dissipates energy via radiation and convection on all surfaces. The sensor is insulated on all surfaces except the top, which is subjected to both convection and radiation. The thermal material properties are set to those of alumina.

The following table summarizes the material properties used in the application:

TABLE 1: MATERIAL PROPERTIES.

MATERIAL	k (W/(m·K))	ρ (kg/m^3)	C_p (J/(kg·K))	ε
IR lamp	400	8700	10	0.99
Silicon wafer (silicon)	163	2330	703	0.5
Sensor	27	2000	500	0.8

The model simulates the transient temperature field for 10 s of heating. The initial temperature is 400 K for all objects.

Results and Discussion

Figure 3 displays the temperature distribution after 10 s of heating.

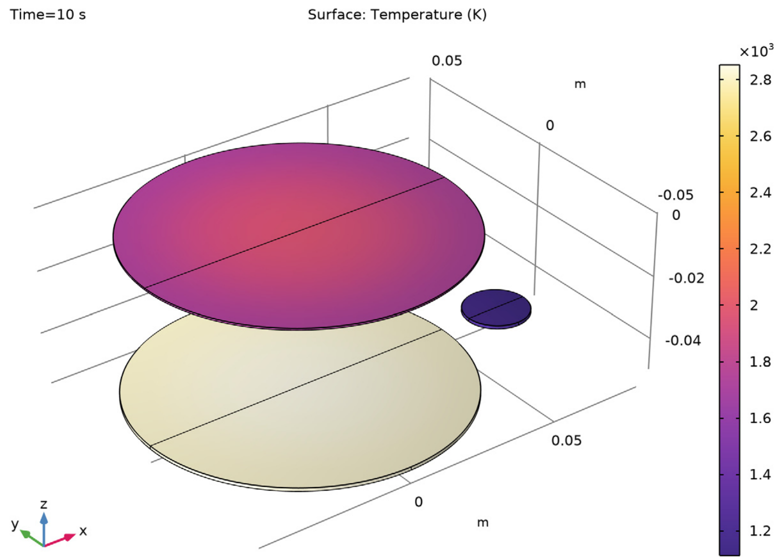


Figure 3: Temperatures of the lamp, wafer, and sensor after 10 s of heating.

After 10 seconds, the temperatures of the wafer and sensor differ significantly: the wafer is close to 2000 K, whereas the sensor is close to 1200 K.

You can notice a delta of several hundred degrees between the center and the periphery of the wafer. A more uniform temperature distribution could be obtained by reconfiguring the heat source, however, such a reconfiguration is not included in this application.

To investigate how well the sensor's temperature reflects that of the wafer surface, it is useful to plot the temperature transient of the wafer surface's centerpoint that faces the lamp (T_{wafer}), together with the temperature at a point on the sensor top surface (T_{sensor}) (see Figure 4).

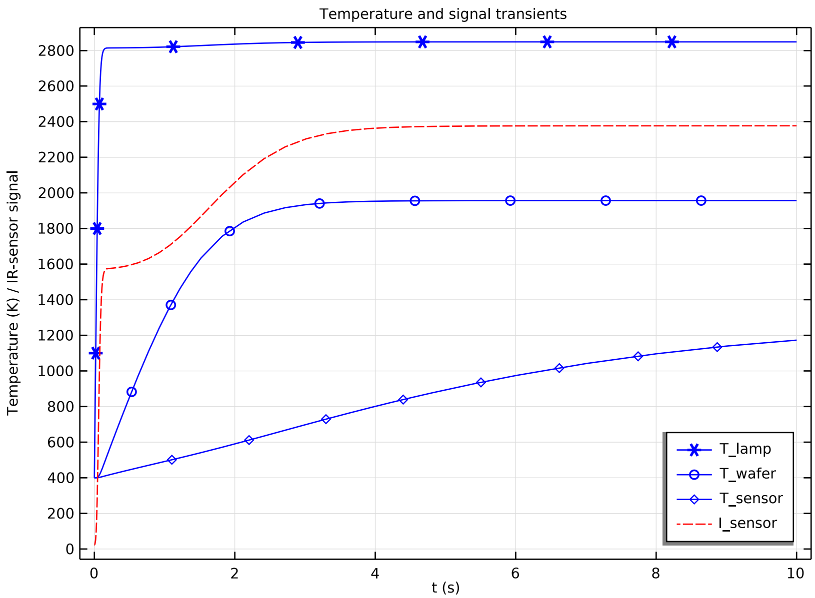


Figure 4: The temperature transients of the lamp, the silicon wafer, and the sensor, together with the irradiation power at the sensor surface.

The sensor temperature reflects that of the silicon wafer poorly. This means that the signal of a thermocouple, positioned anywhere in the sensor domain of Figure 2, is of little use for regulating this process.

The IR-detector transient (I_{sensor}) matches the wafer temperature characteristic quite well. A scalar amplification allows for a high accuracy measurement of the wafer temperature. The precise amplification factor is system-dependent and subject to a calibration requirement.

However, IR-sensor methodology also has drawbacks. The IR signal depends on the emissivity of the wafer, which varies with temperature making the response nonlinear. Furthermore, the IR signal is very sensitive to geometry changes.

The bright side is that COMSOL Multiphysics does not set any limits with respect to these phenomena and allows you to study them fully.

Reference

1. A.T. Fiory, "Methods in Rapid Thermal Annealing," *Proc. 8th Int'l Conf. Advanced Thermal Processing of Semiconductors* (RTP 2000).

Application Library path: `Heat_Transfer_Module/Thermal_Radiation/thermal_annealing`

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 **Heat Transfer>Radiation>Heat Transfer with Surface-to-Surface Radiation**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

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
T_wall	400[K]	400 K	Temperature, wall
T_gas	400[K]	400 K	Temperature, gas
h_gas	20[W/(m^2*K)]	20 W/(m²·K)	Heat transfer coefficient

Name	Expression	Value	Description
k_sens	27[W/(m*K)]	27 W/(m·K)	Thermal conductivity, sonsor
rho_sens	2000[kg/m^3]	2000 kg/m³	Density, sensor
Cp_sens	500[J/(kg*K)]	500 J/(kg·K)	Heat capacity, sensor
e_sens	0.8	0.8	Surface emissivity, sensor
k_lamp	400[W/(m*K)]	400 W/(m·K)	Thermal conductivity, lamp
rho_lamp	8700[kg/m^3]	8700 kg/m³	Density, lamp
Cp_lamp	10[J/(kg*K)]	10 J/(kg·K)	Heat capacity, lamp
e_lamp	0.99	0.99	Surface emissivity, lamp
P_lamp	25[kW]	25000 W	Total power, lamp
e_wafer	0.5	0.5	Surface emissivity, wafer
ampl	50	50	Amplification factor, IR sensor

COMPONENT 1 (COMP1)

Set the geometric shape order to "Quadratic". By default, the geometric shape order is set to linear in this model. Although the difference will not be visible when plotting the mesh (for graphics performance purposes), second-order elements will then be allowed, yielding a much better match between the mesh and the real cylindrical geometry thanks to the curved edges of the boundary elements.

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

2 In the **Settings** window for **Component**, locate the **Curved Mesh Elements** section.

3 From the **Geometry shape function** list, choose **Quadratic Lagrange**.

GEOMETRY 1

Cylinder 1 (cyl1)

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

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

3 In the **Radius** text field, type `0.05`.

4 In the **Height** text field, type `5e-4`.

5 Click **Build Selected**.

Cylinder 2 (cyl2)

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

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

3 In the **Radius** text field, type `0.05`.

4 In the **Height** text field, type `1e-3`.

5 Locate the **Position** section. In the **z** text field, type `-5e-2`.

6 Click **Build Selected**.

Cylinder 3 (cyl3)

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

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

3 In the **Radius** text field, type `0.01`.

4 In the **Height** text field, type `1e-3`.

5 Locate the **Position** section. In the **x** text field, type `0.07`.

6 In the **z** text field, type `-5e-2`.

7 Click **Build Selected**.

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

The built geometry shows a plane symmetry. Delete half of it to optimize the computation.

Block 1 (blk1)

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 `0.2`.

4 In the **Depth** text field, type `0.2`.

5 In the **Height** text field, type `0.2`.

6 Locate the **Position** section. In the **x** text field, type `-0.1`.

7 In the **y** text field, type `-0.2`.

8 In the **z** text field, type `-0.1`.

9 Click **Build Selected**.

Difference 1 (dif1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

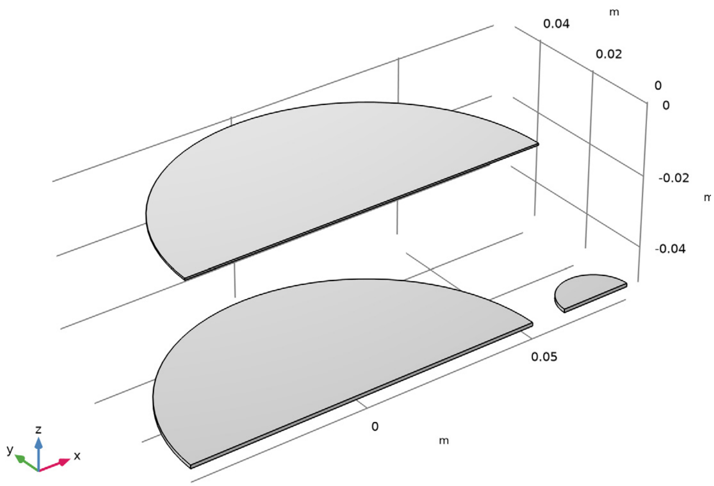
2 Select the objects **cyl1**, **cyl2**, and **cyl3** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Find the **Objects to subtract** subsection. Click to select the **Activate Selection** toggle button.

5 Select the object **blk1** only.

6 Click **Build Selected**.



7 In the **Geometry** toolbar, click **Build All**.

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

In preparation for analyzing and visualizing the results, define a nonlocal integration coupling.

DEFINITIONS

Integration 1 (intop1)

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

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

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

4 Select Boundary 14 only.

Variables 1

1 In the **Definitions** toolbar, click a= **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
`I_sens`	`2*intop1(rad.Grad)`	W	`Irradiated heat effect, sensor`

`ht.G_rad` is a predefined physics interface variable representing inward radiation, which includes both surface-to-surface and surface-to-ambient contributions.

The integral is multiplied by 2 to get the irradiated heat effect on the full geometry.

MATERIALS

IR Lamp

1 In the **Materials** toolbar, click **Blank Material**.

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

3 Select Domain 1 only.

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`k_lamp`	W/(m·K)	Basic
Density	rho	`rho_lamp`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`Cp_lamp`	J/(kg·K)	Basic

ADD MATERIAL

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

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

3 In the tree, select **Built-in>Silicon**.

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

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

MATERIALS

Silicon (mat2)

Select Domain 2 only.

Sensor

1 In the **Materials** toolbar, click **Blank Material**.

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

3 Select Domain 3 only.

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`k_sens`	W/(m·K)	Basic
Density	rho	`rho_sens`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`Cp_sens`	J/(kg·K)	Basic

Now add materials on the boundaries for the specification of surface emissivities.

IR Lamp (Boundaries)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** right-click **IR Lamp (mat1)** and choose **Duplicate**.

2 In the **Settings** window for **Material**, type `IR Lamp (Boundaries)` in the **Label** text field.

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

4 Select Boundary 4 only.

5 Locate the **Material Properties** section. In the **Material properties** tree, select **Basic Properties>Surface Emissivity**.

6 Click + **Add to Material**.

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

Property	Variable	Value	Unit	Property group
Surface emissivity	epsilon_rad	`e_lamp`	1	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`k_lamp`	W/(m·K)	Basic
Density	rho	`rho_lamp`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`Cp_lamp`	J/(kg·K)	Basic

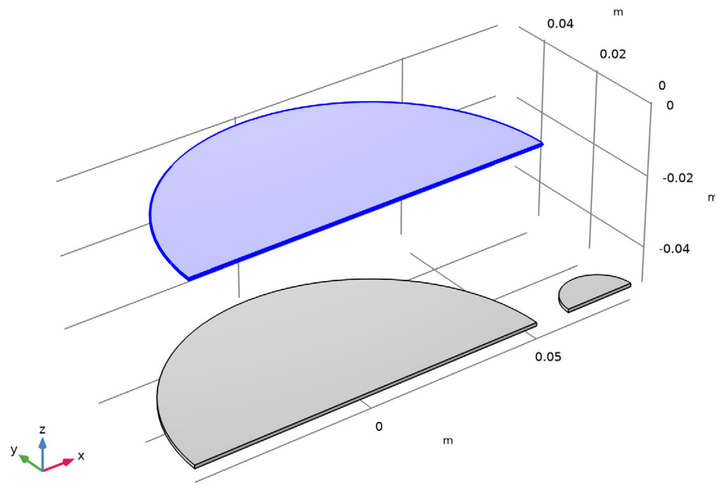
Silicon (Boundaries)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** right-click **Silicon (mat2)** and choose **Duplicate**.

2 In the **Settings** window for **Material**, type `Silicon (Boundaries)` in the **Label** text field.

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

4 Select Boundaries 5, 7, 8, and 10 only.



5 Locate the **Material Properties** section. In the **Material properties** tree, select **Basic Properties>Surface Emissivity**.

6 Click **Add to Material**.

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

Property	Variable	Value	Unit	Property group
Surface emissivity	epsilon_rad	`e_wafer`	1	Basic
Relative permeability	mur_iso ; murii = mur_iso, murij = 0	`700[J/(kg*K)]`	1	Basic
Electrical conductivity	sigma_iso ; sigmaii = sigma_iso, sigmaij = 0	`2329[kg/m^3]`	S/m	Basic

Property	Variable	Value	Unit	Property group
Coefficient of thermal expansion	alpha_iso ; alphaii = alpha_iso, alphaij = 0	130[W/(m*K)]	1/K	Basic
Heat capacity at constant pressure	Cp	1	J/(kg·K)	Basic
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	1e-12[S/m]	1	Basic
Density	rho	2.6e-6[1/K]	kg/m³	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	11.7	W/(m·K)	Basic
Young's modulus	E	170e9[Pa]	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	nu	0.28	1	Young's modulus and Poisson's ratio
Refractive index, real part	n_iso ; nii = n_iso, nij = 0	3.48	1	Refractive index
Refractive index, imaginary part	ki_iso ; kiii = ki_iso, kiij = 0	0	1	Refractive index

Sensor (Boundaries)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** right-click **Sensor (mat3)** and choose **Duplicate**.

2 In the **Settings** window for **Material**, type `Sensor (Boundaries)` in the **Label** text field.

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

4 Select Boundary 14 only.

5 Locate the **Material Properties** section. In the **Material properties** tree, select **Basic Properties>Surface Emissivity**.

6 Click + **Add to Material**.

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

Property	Variable	Value	Unit	Property group
Surface emissivity	epsilon_rad	e_sens	1	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	k_sens	W/(m·K)	Basic
Density	rho	rho_sens	kg/m³	Basic
Heat capacity at constant pressure	Cp	Cp_sens	J/(kg·K)	Basic

HEAT TRANSFER IN SOLIDS (HT)

Heat Source 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Heat Transfer in Solids (ht)** and choose **Heat Source**.

2 Select Domain 1 only.

3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.

4 From the **Heat source** list, choose **Heat rate**.

Define the total power as half of the lamp power on the reduced geometry.

5 In the P_0 text field, type `P_lamp/2`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `T_wall`.

Heat Flux 1

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

2 Select Boundaries 5, 7, 8, 10, and 14 only.

3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.

4 From the **Flux type** list, choose **Convective heat flux**.

5 In the h text field, type `h_gas`.

6 In the T_{ext} text field, type `T_gas`.

Symmetry 1

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

2 Select Boundaries 2, 6, and 12 only.

With the **Symmetry** feature, only the symmetry of the temperature field is handled. To consider also symmetry for radiation computation, add a **Symmetry for Surface-to-Surface Radiation** feature.

SURFACE-TO-SURFACE RADIATION (RAD)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Surface-to-Surface Radiation (rad)**.

2 Select Boundaries 4, 5, 7, 8, 10, and 14 only.

Diffuse Surface 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Surface-to-Surface Radiation (rad)** click **Diffuse Surface 1**.

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

3 In the T_{amb} text field, type `T_wall`.

By default, the radiation direction is controlled by the opacity of the domains. The solid parts are automatically defined as opaque while the fluid parts are transparent. You can change this setting using the **Opacity** feature in the **Surface-to-Surface Radiation** interface.

Symmetry for Surface-to-Surface Radiation 1

1 In the **Physics** toolbar, click **Global** and choose **Symmetry for Surface-to-Surface Radiation**.

2 In the **Settings** window for **Symmetry for Surface-to-Surface Radiation**, locate the **Plane Symmetry** section.

3 From the **Selection method** list, choose **Point selection**.

4 Locate the **First Point Defining Reflection Plane** section. Click to select the **Activate Selection** toggle button.

5 Select Point 1 only.

6 Locate the **Second Point Defining Reflection Plane** section. Click to select the **Activate Selection** toggle button.

7 Select Point 3 only.

8 Locate the **Third Point Defining Reflection Plane** section. Click to select the **Activate Selection** toggle button.

9 Select Point 9 only.

MESH 1

Free Triangular 1

In the **Mesh** toolbar, click **Boundary** and choose **Free Triangular**.

Size

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

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

3 From the **Predefined** list, choose **Finer**.

Free Triangular 1

1 In the **Model Builder** window, click **Free Triangular 1**.

2 Select Boundaries 4, 8, and 14 only.

Swept 1

1 In the **Mesh** toolbar, click **Swept**.

2 In the **Settings** window for **Swept**, click **Build All**.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

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

3 In the **Output times** text field, type `0 10`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1e-3`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Output** section.

4 Locate the **General** section. From the **Times to store** list, choose **Steps taken by solver**.

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

RESULTS

Temperature (ht)

1 In the **Temperature (ht)** toolbar, click **Plot**.

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

The first default 3D plot shows the temperature at the final time step on half of the full geometry. To visualize the temperature on the full geometry, define a new dataset.

Mirror 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 3D**.

2 In the **Settings** window for **Mirror 3D**, locate the **Plane Data** section.

3 From the **Plane** list, choose **ZX-planes**.

4 Click **Plot**.

Temperature (ht)

1 In the **Model Builder** window, under **Results** click **Temperature (ht)**.

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

3 From the **Dataset** list, choose **Mirror 3D 1**.

4 In the **Temperature (ht)** toolbar, click **Plot**.

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

You can now see the plot of Figure 3.

Two other default plots show isothermal contours and radiosity.

Reproduce the plots in Figure 4 with the following steps:

Cut Point 3D 1

1 In the **Results** toolbar, click **Cut Point 3D**.

2 In the **Settings** window for **Cut Point 3D**, locate the **Point Data** section.

3 In the **X** text field, type `0, 0, 0.06`.

4 In the **Y** text field, type `0`.

5 In the **Z** text field, type `-0.049, 0, -0.049`.

Temperature and Signal Transients

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

2 In the **Settings** window for **1D Plot Group**, type `Temperature and Signal Transients` in the **Label** text field.

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

4 In the **Title** text area, type `Temperature and signal transients`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `t (s)`.

7 Select the **y-axis label** check box. In the associated text field, type `Temperature (K) / IR-sensor signal`.

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

Point Graph 1

1 In the **Temperature and Signal Transients** toolbar, click **Point Graph**.

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

3 From the **Dataset** list, choose **Cut Point 3D 1**.

4 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Blue**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

6 From the **Positioning** list, choose **Interpolated**.

7 Click to expand the **Legends** section. Select the **Show legends** check box.

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

9 In the table, enter the following settings:

Legends
T_lamp
T_wafer
T_sensor

Temperature and Signal Transients

In the **Model Builder** window, click **Temperature and Signal Transients**.

Global 1

1 In the **Temperature and Signal Transients** toolbar, click **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
I_sens*ampl	W	

4 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Red**.

5 Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

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

7 In the table, enter the following settings:

Legends
`I_sensor`

8 In the **Temperature and Signal Transients** toolbar, click **Plot**.