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 depicted in Figure 1, uses high-power IR lamps as heat sources (Ref. 1).

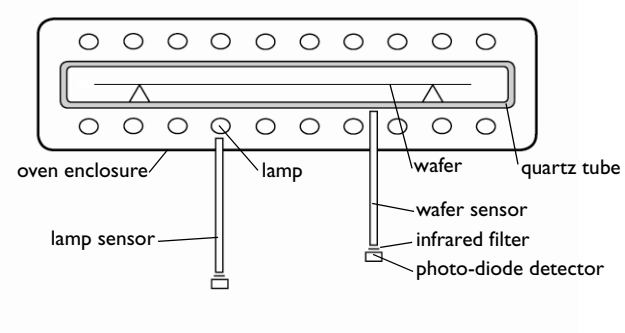

Figure 1: Diagram of a typical RTA (rapid thermal annealing) apparatus.

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 not be 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 depicted in Figure 2.

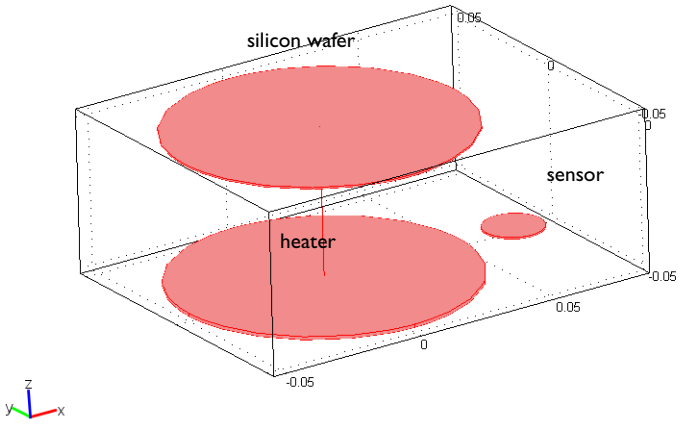

Figure 2: The model geometry.

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:

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

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

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 for 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 at 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 model:

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.

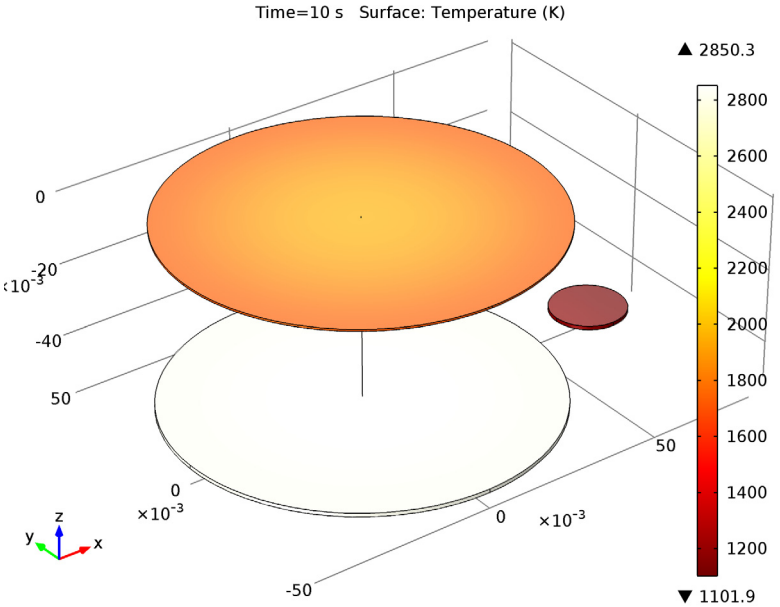

Figure 3: Temperatures of the lamp, wafer, and sensor after 10 s of heating.

After 10 seconds, the temperatures of the wafer and sensor differ significantly: the wafer is at 1800 K, whereas the sensor is at 1100 K.

Notice that the temperature distribution in the wafer with a delta of several hundred degrees is not very uniform, and that you probably can do much better by reconfiguring the heat source. However, such a reconfiguration is not included in this model.

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).

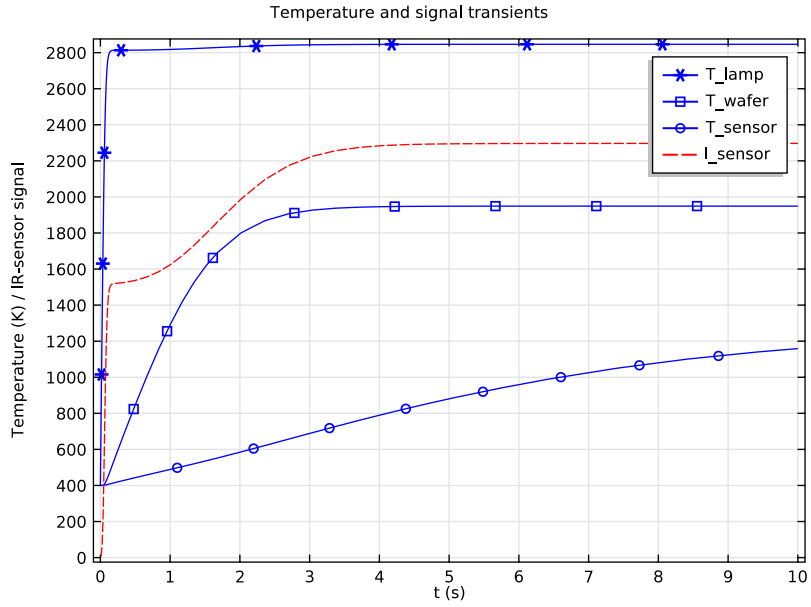

Figure 4: The temperature transients of the lamp, the silicon wafer, and the sensor, together with the irradiation power at the sensor surface.

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 ($\mathrm{Sens}_{\mathrm{irrad}}$) 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 will vary 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), http://web.njit.edu/~fiory/Papers/RapidThermalAnnealing00.pdf, pp. 15–25.

Model Library path: `Heat_Transfer_Module/Thermal_Radiation/thermal_annealing`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click the **3D** button.

2 In the **Select physics** tree, select **Heat Transfer>Radiation>Heat Transfer with Surface-to-Surface Radiation (ht)**.

3 Click the **Add** button.

4 Click the **Study** button.

5 In the tree, select **Preset Studies>Time Dependent**.

6 Click the **Done** button.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
T_wall	400[K]	400.0 K	Temperature, wall
T_gas	400[K]	400.0 K	Temperature, gas

Name	Expression	Value	Description
h_gas	20[W/(m^2*K)]	20.00 W/(m²·K)	Heat transfer coefficient
k_sens	27[W/(m*K)]	27.00 W/(m·K)	Thermal conductivity, sonsor
rho_sens	2000[kg/m^3]	2000 kg/m³	Density, sensor
Cp_sens	500[J/(kg*K)]	500.0 J/(kg·K)	Heat capacity, sensor
e_sens	0.8	0.8000	Surface emissivity, sensor
k_lamp	400[W/(m*K)]	400.0 W/(m·K)	Thermal conductivity, lamp
rho_lamp	8700[kg/m^3]	8700 kg/m³	Density, lamp
Cp_lamp	10[J/(kg*K)]	10.00 J/(kg·K)	Heat capacity, lamp
e_lamp	0.99	0.9900	Surface emissivity, lamp
P_lamp	25[kW]	25[kW]	Total power, lamp
e_wafer	0.5	0.5000	Surface emissivity, wafer
ampl	50	50.00	Amplification factor, IR sensor

GEOMETRY 1

Cylinder 1

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

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

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

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

5 Click the **Build Selected** button.

Cylinder 2

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

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

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

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

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

6 Click the **Build Selected** button.

Cylinder 3

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

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

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

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

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

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

7 Click the **Build All Objects** button.

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

MATERIALS

Material 1

1 In the **Model Builder** window, under **Component 1** right-click **Materials** and choose **New Material**.

2 Select Domain 1 only.

3 In the **Material** settings window, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	`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

5 Right-click **Component 1>Materials>Material 1** and choose **Rename**.

6 Go to the **Rename Material** dialog box and type `IR lamp` in the **New name** edit field.

7 Click **OK**.

8 On the **Home** toolbar, click **Add Material**.

ADD MATERIAL

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

2 In the tree, select **Built-In>Silicon**.

3 In the **Add material** window, click **Add to Component**.

MATERIALS

Silicon

1 In the **Model Builder** window, under **Component 1>Materials** click **Silicon**.

2 Select Domain 2 only.

Material 3

1 In the **Model Builder** window, right-click **Materials** and choose **New Material**.

2 Select Domain 3 only.

3 In the **Material** settings window, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	`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

5 Right-click **Component 1>Materials>Material 3** and choose **Rename**.

6 Go to the **Rename Material** dialog box and type `Sensor` in the **New name** edit field.

7 Click **OK**.

HEAT TRANSFER WITH SURFACE-TO-SURFACE RADIATION

Heat Source 1

1 On the **Physics** toolbar, click **Domains** and choose **Heat Source**.

2 Select Domain 1 only.

3 In the **Heat Source** settings window, locate the **Heat Source** section.

4 Click the **Total power** button.

5 In the P_{tot} edit field, type `P_lamp`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1>Heat Transfer with Surface-to-Surface Radiation** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

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

Heat Flux 1

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

2 Select Boundaries 5–8, 10, 12, and 16 only.

3 In the **Heat Flux** settings window, locate the **Heat Flux** section.

4 Click the **Inward heat flux** button.

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

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

Surface-to-Surface Radiation 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Surface-to-Surface Radiation**.

2 Select Boundary 4 only.

3 In the **Surface-to-Surface Radiation** settings window, locate the **Ambient** section.

4 In the T_{amb} edit field, type `T_wall`.

5 Locate the **Surface Emissivity** section. From the ε list, choose **User defined**. In the associated edit field, type `e_lamp`.

By default the radiation direction is controlled by the opacity of the domains. The solid parts are automatically defined as opaque. You can change this setting by adding or modifying **Opaque** subnodes under the **Heat Transfer in Solids** node.

Surface-to-Surface Radiation 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Surface-to-Surface Radiation**.

2 Select Boundary 16 only.

3 In the **Surface-to-Surface Radiation** settings window, locate the **Ambient** section.

4 In the T_{amb} edit field, type `T_wall`.

5 Locate the **Surface Emissivity** section. From the ε list, choose **User defined**. In the associated edit field, type `e_sens`.

Surface-to-Surface Radiation 3

1 On the **Physics** toolbar, click **Boundaries** and choose **Surface-to-Surface Radiation**.

2 Select Boundary 7 only.

3 In the **Surface-to-Surface Radiation** settings window, locate the **Ambient** section.

4 In the T_{amb} edit field, type `T_wall`.

5 Locate the **Surface Emissivity** section. From the ε list, choose **User defined**. In the associated edit field, type `e_wafer`.

Surface-to-Ambient Radiation 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Surface-to-Ambient Radiation**.

2 Select Boundaries 5, 6, 8, 10, and 12 only.

3 In the **Surface-to-Ambient Radiation** settings window, locate the **Surface-to-Ambient Radiation** section.

4 From the ε list, choose **User defined**. In the associated edit field, type `e_wafer`.

5 In the T_{amb} edit field, type `T_wall`.

MESH 1

Free Tetrahedral 1

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

2 In the **Free Tetrahedral** settings window, click to expand the **Scale geometry** section.

3 Locate the **Scale Geometry** section. In the **z-direction scale** edit field, type `5`.

Size

1 In the **Model Builder** window, under **Component 1>Mesh 1** click **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra coarse**.

4 Click the **Build All** button.

DEFINITIONS

In preparation for analyzing and visualizing the results, define an integration coupling operator. In addition, a line intersecting the lamp and wafer surfaces will also be useful.

Integration 1

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

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

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

4 Select Boundary 16 only.

Variables 1

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Variables** settings window, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
I_sens	intop1(ht.Gm)	W	Irradiated heat effect, sensor

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

GEOMETRY 1

Bézier Polygon 1

1 On the **Geometry** toolbar, click **More Primitives** and choose **Bézier Polygon**.
2 In the **Bézier Polygon** settings window, locate the **Polygon Segments** section.
3 Find the **Added segments** subsection. Click the **Add Linear** button.
4 Find the **Control points** subsection. In row **1**, set **z** to `-5e-2`.
5 In row **2**, set **z** to `1e-3`.
6 Click the **Build All Objects** button.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.
2 In the **Time Dependent** settings window, locate the **Study Settings** section.
3 In the **Times** edit field, type `0 10`.
4 Select the **Relative tolerance** check box.
5 In the associated edit field, type `0.001`.

Solver 1

1 On the **Study** toolbar, click **Show Default Solver**.
2 In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.
3 In the **Model Builder** window, expand the **Solver 1** node, then click **Time-Dependent Solver 1**.
4 In the **Time-Dependent Solver** settings window, click to expand the **Output** section.
5 From the **Times to store** list, choose **Steps taken by solver**.
6 On the **Home** toolbar, click **Compute**.

RESULTS

Temperature (ht)

1 On the **3D plot group** toolbar, click **Plot**.

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

The first default 3D plot shows the temperature at the final time step (Figure 3).

Two others default plots show isothermal contours and radiosity.

Reproduce the plots in Figure 4 with the following steps:

1D Plot Group 4

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

2 In the **1D Plot Group** settings window, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

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

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated edit field, type `t (s)`.

7 Select the **y-axis label** check box.

8 In the associated edit field, type `Temperature (K) / IR-sensor signal`.

9 On the **1D plot group** toolbar, click **Point Graph**.

10 Select Point 10 only.

11 In the **Point Graph** settings window, click to expand the **Coloring and style** section.

12 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Color** list, choose **Blue**.

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

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

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

16 In the table, enter the following settings:

Legends
T_lamp

17 On the **1D plot group** toolbar, click **Point Graph**.

18 Select Point 11 only.

19 In the **Point Graph** settings window, locate the **Coloring and Style** section.

20 Find the **Line style** subsection. From the **Color** list, choose **Blue**.

21 Find the **Line markers** subsection. From the **Marker** list, choose **Square**.

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

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

24 In the table, enter the following settings:

Legends
T_wafer

25 On the **1D plot group** toolbar, click **Point Graph**.

26 Select Point 23 only.

27 In the **Point Graph** settings window, locate the **Coloring and Style** section.

28 Find the **Line style** subsection. From the **Color** list, choose **Blue**.

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

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

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

32 In the table, enter the following settings:

Legends
T_sensor

33 On the **1D plot group** toolbar, click **Global**.

34 In the **Global** settings window, locate the **y-Axis Data** section.

35 In the table, enter the following settings:

Expression	Unit	Description
I_sens*ampl	W	

36 Click to expand the **Coloring and style** section. Find the **Line style** subsection. From the **Color** list, choose **Red**.

37 Find the **Line markers** subsection. From the **Line** list, choose **Dashed**.

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

39 In the table, enter the following settings:

Legends
I_sensor

40 On the **1D plot group** toolbar, click **Plot**.

41 In the **Model Builder** window, right-click **1D Plot Group 4** and choose **Rename**.

42 Go to the **Rename 1D Plot Group** dialog box and type `Temperature and signal transients` in the **New name** edit field.

43 Click **OK**.