Molecular Flow in an Ion-Implant Vacuum System

Introduction

This example considers the design of an ion implantation system. Ion implantation is used extensively in the semiconductor industry to implant dopants into wafers. Within an ion implanter ions generated within an ion source are accelerated by an electric field to achieve the desired implant energy. Ions of the correct charge state are selected by means of a separation magnet which bends the ion beam to ensure that ions of a particular charge to mass ratio are the only ones which reach the wafer. The energy dose and angle of the ion beam are both key parameters for the process. This part of the system is known as the corrector.

Usually it is desired that only selected regions of the wafer are implanted. This is achieved by masking parts of the wafer with an organic photoresist, to produce the desired pattern. Unfortunately, the photoresist itself emits gas molecules as a result of the beam striking it. These molecules can interact with the ion beam and produce species with undesired charge to mass ratios at different points along the beam path. Some of these species may reach the wafer, degrading the uniformity of the implant, which is highly undesirable. Additionally, these ions may also effect the accuracy of measurements of the implant dose. A key requirement for the system is that the number density of the outgassing molecules for the wafer is low within the beam line.

This example shows how to model an ion implantation system using the Molecular Flow interface. Because it is interactions of outgassing molecules with the beam that produce undesirable species, the average number density of these molecules along the beam path is used as a figure of merit to evaluate the design. Furthermore, because the angle of the wafer to the beam can be modified, the figure of merit must be computed as a function of wafer angle, with rotation about one axis.

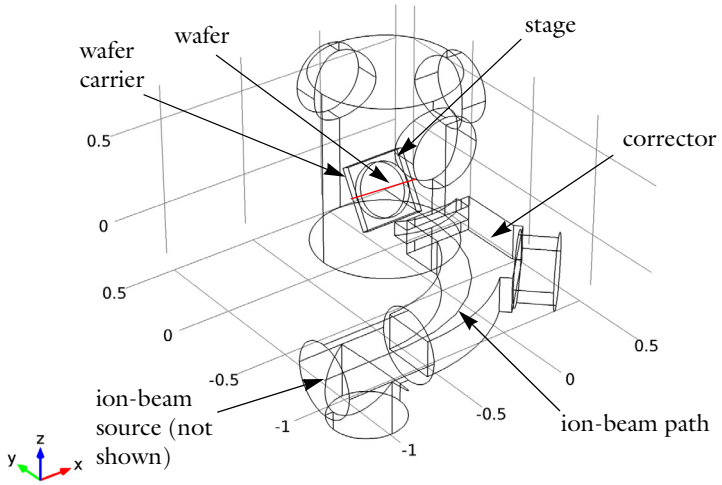


Figure 1: Model geometry. Key components of the system are labeled. The red line through he center of the wafer carrier indicates the axis of rotation of the carrier.

Note: This model is motivated by Ref. 1. However, it is important to note that there are significant differences between the pressure and number density computed by COMSOL's Molecular flow interface and those computed in the radiation analogy, which is used in Ref. 1. COMSOL computes these quantities accurately, whilst the radiation analogy uses an approximate technique to compute the number density and pressure which can result in misleading, incorrect, answers.

Model Definition

The model geometry is shown in Figure 1. The wafer is positioned on a carrier plate which is rotated about an axis through its center to achieve different implant angles. The carrier plate is mounted in a chamber that is pumped by three large cryopumps, on cylindrical vacuum ports. These pumps have a pump speed of 12,000 l/s. In this model outgassing of only one species from the wafer (H_2) is considered: multiple species can be modeled by adding additional molecular flow interfaces. It is assumed that the outgassing across the wafer surface is uniform and that the total gas emitted is 30 sccm. The vacuum path through the corrector magnetic field enters the main

chamber opposite the wafer, and is pumped by a turbo-molecular pump on a cylindrical port midway down the corrector, with a pump speed of 1500 l/s and an additional cryopump at the start of the beam path, with a pump speed of 12,000 l/s. There is an aperture at the entrance to the chamber which reduces the flux that enters the corrector. The angle of the wafer normal to the ion beam is swept from 0° to 60° in 20° steps, as the wafer is rotated about the horizontal axis through its center, as shown in Figure 1. All other surfaces in the model are walls.

Results and Discussion

The molecular flux at the surfaces of the vacuum chamber is shown in Figure 2, for wafer normal angles of 0° and 40° to the beam.

The shadowing effect of the wafer support is evident at both wafer angles shown in Figure 2. It is also clear that more flux enters the beam line when the wafer normal is parallel to the beam, because the line of sight with the beam line is then parallel to the wafer normal. The number density along the beam path is shown in Figure 3, for each of the angles solved for. The number density increases along the beam path towards the wafer, with strong changes in gradient as the beam passes through different apertures. Note that in the immediate vicinity of the wafer the number density is not computed accurately (this is difficult to see from the plot below, but zooming into the plot at the end of the beam shows issues in the results for elements adjacent to the surface). This is a result of numerical issues when computing the number density very close to a source surface within the domain.

The average number density along the beam path within the corrector can be used as figure of merit for the system design. This quantity is plotted against the angle of the wafer normal to the beam line in Figure 4. The average flux in the corrector is reduced by rotating the wafer normal away from the beam line with a 10% reduction occurring over the full angular range. Rotating the wafer in this manner can therefore result in improved performance of the implanter.

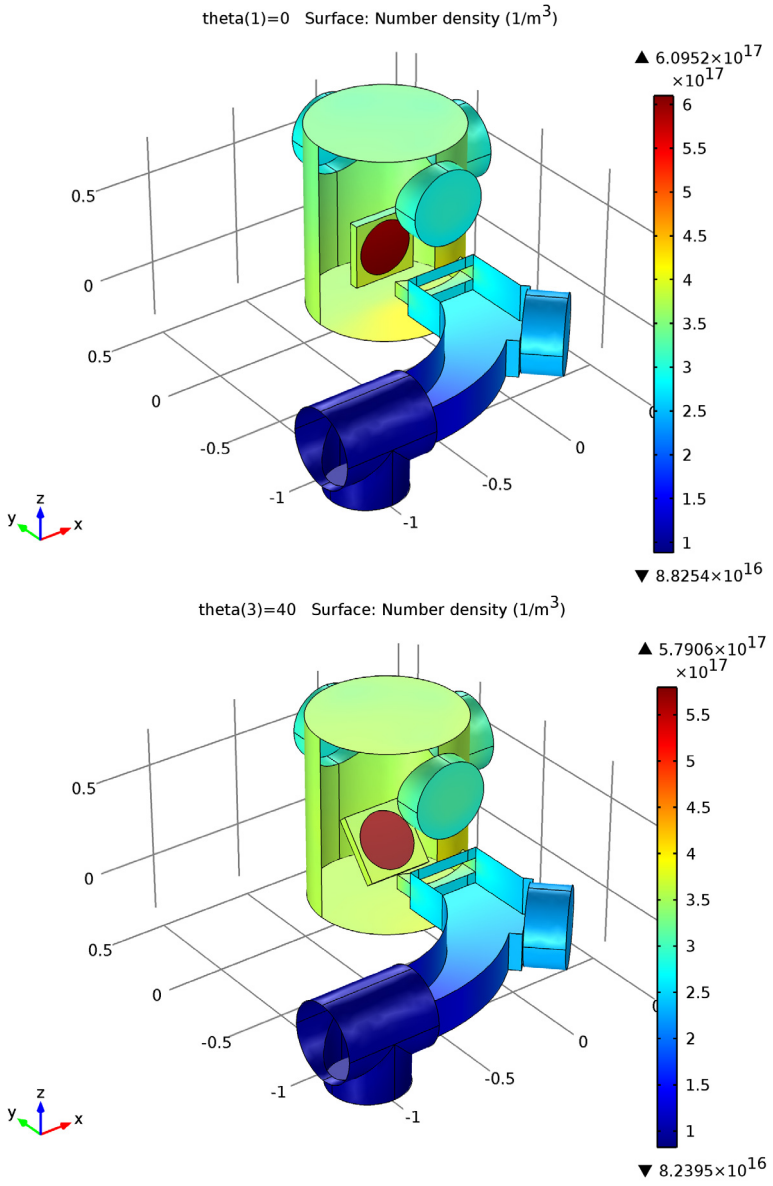


Figure 2: Pressure on the surface of the ion implanter, with the wafer normal at 0° (top) and 40° (bottom) to the beam path.

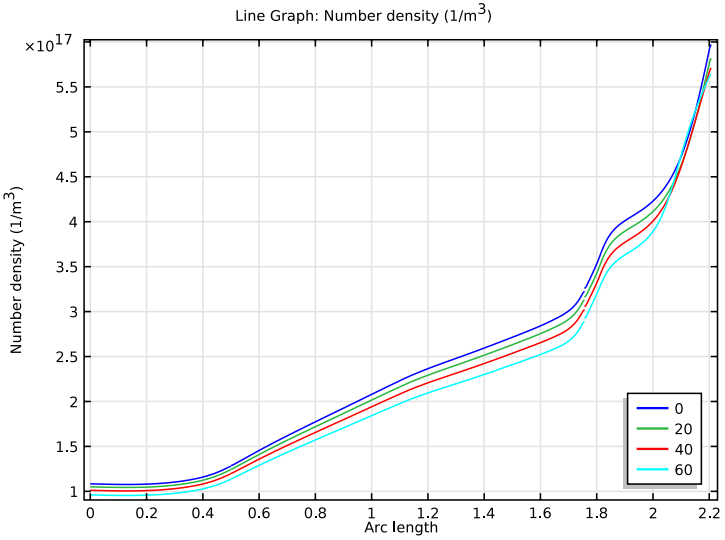


Figure 3: The number density as a function of position along the beam line.

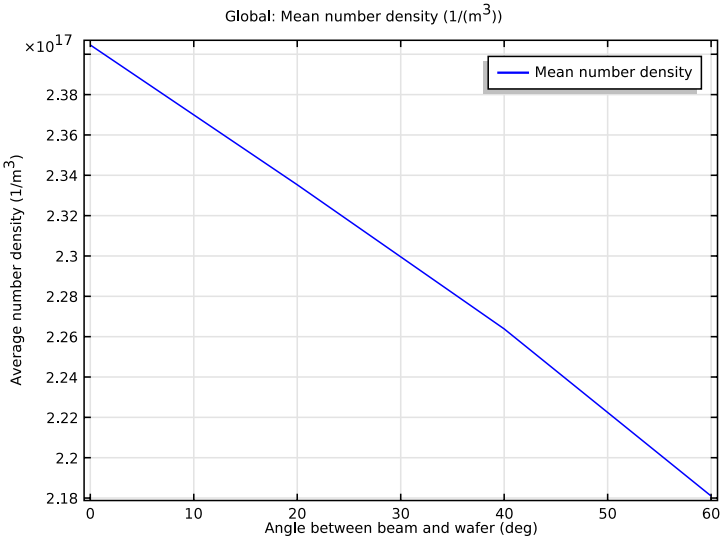


Figure 4: Plot of the average number density along the beam line as a function of the wafer normal angle to the incoming beam.

Reference

1. M.R. LaFontaine, N. Tokoro, P. Murphy, and D. Holbrook, "Modelling Photoresist Outgassing Pressure Distribution Using the Finite Element Method," *Proc. Conference on Ion Implantation Technology*, IEEE Press, pp. 247–250, 2000.

Notes About the COMSOL Implementation

The model is straightforward to set up using the Molecular Flow interface. The vacuum pump boundary condition is used for the pumps and the outgassing wall boundary condition is used for the wafer surface. The geometry for the vacuum system is imported, but the wafer and its carrier are generated within COMSOL Multiphysics so that the angle to the beam line can be easily parameterized.

Model Library path: `Molecular_Flow_Module/Industrial_Models/ion_implanter`

Modeling Instructions

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 **Fluid Flow>Rarefied Flow>Free Molecular Flow (fmf)**.

3 Click the **Add** button.

4 Click the **Study** button.

5 In the tree, select **Preset Studies>Stationary**.

6 Click the **Done** button.

GLOBAL DEFINITIONS

Set up parameters for the wafer angle and pump speeds.

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
theta	30	30.00	Wafer angle
pumpspeed cryo	12000[l/s]	12.00 m³/s	Pump speed for cryo-pumps
pumpspeed turbo	1500[l/s]	1.500 m³/s	Pump speed for turbo-pump

GEOMETRY 1

Import the ion implanter chamber geometry.

Import 1

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

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

3 Click the **Browse** button.

4 Browse to the model's Model Library folder and double-click the file `ion_implanter.mphbin`.

5 Click the **Import** button.

Next add the wafer and carrier geometry to the model.

6 In the **Model Builder** window, click **Geometry 1**.

7 In the **Geometry** settings window, locate the **Units** section.

8 From the **Angular unit** list, choose **Radians**.

Work Plane 1

1 On the **Geometry** toolbar, click **Work Plane**.

2 In the **Work Plane** settings window, locate the **Plane Definition** section.

3 From the **Plane type** list, choose **Coordinates**.

4 In row **Point 3**, set **y** to `sin(theta[deg])`.

5 In row **Point 3**, set **z** to `cos(theta[deg])`.

Circle 1

1 In the **Model Builder** window, under **Component 1>Geometry 1>Work Plane 1** right-click **Plane Geometry** and choose **Circle**.

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

3 In the **Radius** edit field, type `0.15`.

Square 1

1 Right-click **Plane Geometry** and choose **Square**.

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

3 In the **Side length** edit field, type `0.35`.

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

5 Click the **Build All** button.

Extrude 1

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

2 In the **Extrude** settings window, locate the **Distances from Plane** section.

3 In the table, enter the following settings:

Distances (m)
0.05

4 Select the **Reverse direction** check box.

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

Difference 1

Subtract the wafer/carrier domain from the chamber domain to produce a single volume for the interior space in the chamber.

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

2 Select the object **imp1** only.

3 In the **Difference** settings window, locate the **Difference** section.

4 Select the **Objects to subtract** toggle button.

5 Select the object **ext1** only.

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

DEFINITIONS

Add an average operator to compute the average number density along the beam line.

Average 1

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

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

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

4 Click the **Wireframe Rendering** button on the Graphics toolbar.

5 Select Edges 6, 33, and 103 only.

FREE MOLECULAR FLOW

Set the physics interface to simulate free molecular flow of hydrogen.

Molecular Flow 1

1 In the **Model Builder** window, expand the **Component 1>Free Molecular Flow** node, then click **Molecular Flow 1**.

2 In the **Molecular Flow** settings window, locate the **Molecular Flow** section.

3 In the M_n edit field, type `0.002[kg/mol]`.

Wall 2

Set up the wafer to outgas 30 sccm of hydrogen.

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

2 Select Boundary 42 only.

3 In the **Wall** settings window, locate the **Wall Type** section.

4 From the **Wall type** list, choose **Outgassing wall**.

5 Locate the **Flux** section. From the **Outgoing flux** list, choose **Number of SCCM units**.

6 In the Q_{sccm} edit field, type `30`.

Vacuum Pump 1

Set up the vacuum pumps.

1 On the **Physics** toolbar, click **Boundaries** and choose **Vacuum Pump**.

2 In the **Vacuum Pump** settings window, locate the **Vacuum Pump** section.

3 From the **Specify pump flux** list, choose **Pump speed**.

4 Select Boundary 55 only.

5 In the S edit field, type `pumpspeedturbo`.

Vacuum Pump 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Vacuum Pump**.

2 In the **Vacuum Pump** settings window, locate the **Vacuum Pump** section.

3 From the **Specify pump flux** list, choose **Pump speed**.

4 Select Boundary 8 only.

5 In the S edit field, type `pumpspeedcryo`.

Vacuum Pump 3

1 Right-click **Component 1>Free Molecular Flow>Vacuum Pump 2** and choose **Duplicate**.

2 In the **Vacuum Pump** settings window, locate the **Boundary Selection** section.

3 Click **Clear Selection**.

4 Select Boundary 25 only.

Vacuum Pump 4

1 Right-click **Component 1>Free Molecular Flow>Vacuum Pump 3** and choose **Duplicate**.

2 In the **Vacuum Pump** settings window, locate the **Boundary Selection** section.

3 Click **Clear Selection**.

4 Select Boundary 69 only.

Vacuum Pump 5

1 Right-click **Component 1>Free Molecular Flow>Vacuum Pump 4** and choose **Duplicate**.

2 In the **Vacuum Pump** settings window, locate the **Boundary Selection** section.

3 Click **Clear Selection**.

4 Select Boundary 33 only.

Number Density Reconstruction 1

1 On the **Physics** toolbar, click **Edges** and choose **Number Density Reconstruction**.

2 Select Edges 6, 33, and 103 only.

MESH 1

Next create the mesh. Add a fine mesh along the beam line.

Edge 1

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

2 Select Edges 6, 33, and 103 only.

Size 1

Use a very fine mesh along the beam line.

1 Right-click **Component 1>Mesh 1>Edge 1** and choose **Size**.

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

5 In the associated edit field, type `0.005`.

Size

Change the global mesh size setting to refine the mesh.

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 fine**.

Free Triangular 1

Add a free triangular surface mesh. This will inherit the global mesh size setting.

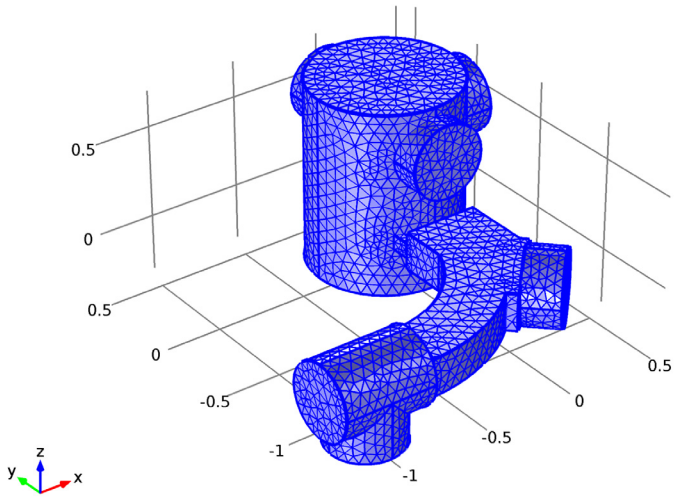
1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Free Triangular** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

4 Click the **Build All** button.

The domain does not need to be meshed since the interface solves equations only on the surfaces of the model. Note that it is possible to mesh sufaces edges and points (as in this model) or to mesh the entire domain. These two approaches cannot be mixed (doing so may lead to incorrect results in some cases).



Set up a parametric sweep over the wafer angle. The study will take approximately 20 minutes to complete with the full sweep. Alternatively it is possible to solve for a single wafer angle to save time.

STUDY 1

Parametric Sweep

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

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

3 Click **Add**.

4 Click **Range**.

5 Go to the **Range** dialog box.

6 In the **Start** edit field, type `0`.

7 In the **Step** edit field, type `20`.

8 In the **Stop** edit field, type `60`.

9 Click the **Add** button.

10 On the **Home** toolbar, click **Compute**.

RESULTS

Create a duplicate solution data set with a selection so that you can see inside the vacuum chamber.

Data Sets

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

2 Right-click **Solution 2** and choose **Duplicate**.

3 Right-click **Results>Data Sets>Solution 3** and choose **Add Selection**.

4 In the **Selection** settings window, locate the **Geometric Entity Selection** section.

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

6 Select Boundaries 2–15, 17, and 19–69 only.

Update the default plots to use the new data set.

Incident Molecular Flux (fmf)

1 In the **Model Builder** window, under **Results** click **Incident Molecular Flux (fmf)**.

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

3 From the **Data set** list, choose **Solution 3**.

Number Density (fmf)

1 In the **Model Builder** window, under **Results** click **Number Density (fmf)**.

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

3 From the **Data set** list, choose **Solution 3**.

Pressure (fmf)

1 In the **Model Builder** window, under **Results** click **Pressure (fmf)**.

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

3 From the **Data set** list, choose **Solution 3**.

Reproduce the results shown in Figure 2.

Number Density (fmf)

1 In the **Model Builder** window, under **Results** click **Number Density (fmf)**.

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

3 From the **Parameter value (theta)** list, choose **0**.

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

Repeat steps 3 and 4, this time selecting an angle of 40 degrees.

Compare the resulting plot with that in Figure 2.

1D Plot Group 4

Create a plot of the number density along the beam path.

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

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

3 From the **Data set** list, choose **Solution 2**.

4 Click to expand the **Legend** section. From the **Position** list, choose **Lower right**.

5 On the **1D plot group** toolbar, click **Line Graph**.

6 Select Edges 6, 33, and 103 only.

7 In the **Line Graph** settings window, click **Replace Expression** in the upper-right corner of the **y-axis data** section. From the menu, choose **Free Molecular Flow>Number density>Number density (fmf.N)**.

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

9 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

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

Compare the resulting plot with that in Figure 3.

1D Plot Group 5

Finally, plot the mean number density along the beam line, as a function of wafer angle.

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

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

3 From the **Data set** list, choose **Solution 2**.

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

5 In the associated edit field, type `Angle between beam and wafer (deg)`.

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

7 In the associated edit field, type `Average number density (1/m<sup>3</sup>)`.

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

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

10 In the table, enter the following settings:

Expression	Unit	Description
`aveop1(fmf.N)`	`1/(m^3)`	`Mean number density`

11 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

12 In the **Expression** edit field, type `theta`.

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

Compare the resulting plot with that in Figure 4.