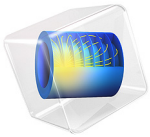

Ion Energy Distribution Function

Introduction

One of the most useful quantities of interest after solving a self-consistent plasma model is the ion energy distribution function (IEDF). The magnitude and shape of the IEDF depends on many of the discharge parameters; pressure, plasma potential, sheath width and so forth. At very low pressures the plasma sheath is said to be collisionless, meaning that the ion energy is not retarded by collisions with the background gas. At higher pressures the ions collide with the background gas molecules in the sheath and their energy at the moment of impact with a surface is reduced.

Note: This application requires the Plasma Module, Particle Tracing Module, and AC/DC Module.

Model Definition

The equations of motion for ions in an electric field and background gas are

$$\frac{d}{dt}(m\mathbf{v}) = qZ\mathbf{E}$$

where m is the ion mass (SI unit: kg), $\mathbf{v}$ is the particle velocity (SI unit: m/s), q is unit charge (SI unit: C), and Z is the ion charge number (SI unit: dimensionless).

When an ion undergoes a collision with the background gas, its velocity vector changes. The probability of a collision event occurring depends in the ion-neutral collision frequency, ν (SI unit: 1/s), which is defined as:

$$\nu = N_d \sigma |\mathbf{v}_p - \mathbf{v}_g|$$

where N_d is the background number density (SI unit: $1/\mathrm{m}^3$), σ is the ion-neutral charge exchange collision cross section (SI unit: m^2), $\mathbf{v}_p$ is the particle velocity, and $\mathbf{v}_g$ is the velocity of the background gas atoms or molecules. In this example the collision cross section is assumed to be constant, $6\text{x}10^{-19}\mathrm{m}^2$, as given in Ref. 2.

The collision probability defined as:

$$P = 1 - \exp(-\nu \Delta t)$$

If P is greater than a random number between 0 and 1 then the particle velocity is reinitialized to the following expression:

$$\mathbf{v}_p' = (m_p\mathbf{v}_p + m_g\mathbf{v}_g - m_g|\mathbf{v}_g - \mathbf{v}_p|\mathbf{R})/(m_p + m_g)$$

where $\mathbf{v}_p$ is the precollision particle velocity, m_g is the mass of the background gas atoms or molecules, $\mathbf{R}$ is a uniformly distributed random unit vector, and $\mathbf{v}_g$ is the velocity of the background gas atoms or molecules, which is sampled from a Maxwellian distribution function:

$$f(\mathbf{v}_g) = \frac{1}{2\pi k_B T/m_g{}^{3/2}} \exp\left[\frac{-(\mathbf{v}_g - \mathbf{u})^2}{(2k_B T)/m_g}\right]$$

where T is the temperature of the background gas.

The particles are released 5 mm away from the wafer surface and 20 mm radially inward from the center of the reactor. There are 22,500 ions modeled. They all start at the same point in space and have an initial Maxwellian distribution function, which is for each velocity direction

$$f(v_i) = \sqrt{\frac{m}{2\pi kT}} \exp\left(-\frac{mv_i^2}{2kT}\right)$$

where T is the initial temperature of the ions, in this case 400 K. This results in a distribution function of

$$\mathbf{f}(\mathbf{v}) = \prod_{i=1}^{\text{nsdim}} f(v_i)$$

When the ions strike the wafer their velocity is frozen for all subsequent time steps. This allows the velocity and energy distribution function to be recovered once all the ions have made contact with the wall.

The angle at which the ions strike the wafer is also of interest. This can be recovered by plotting a histogram of the inverse tangent of the radial and axial particle velocities.

The electric potential for an argon plasma at an operating pressure of 20 mTorr is plotted in Figure 1. The initial starting position for the ions is also shown:

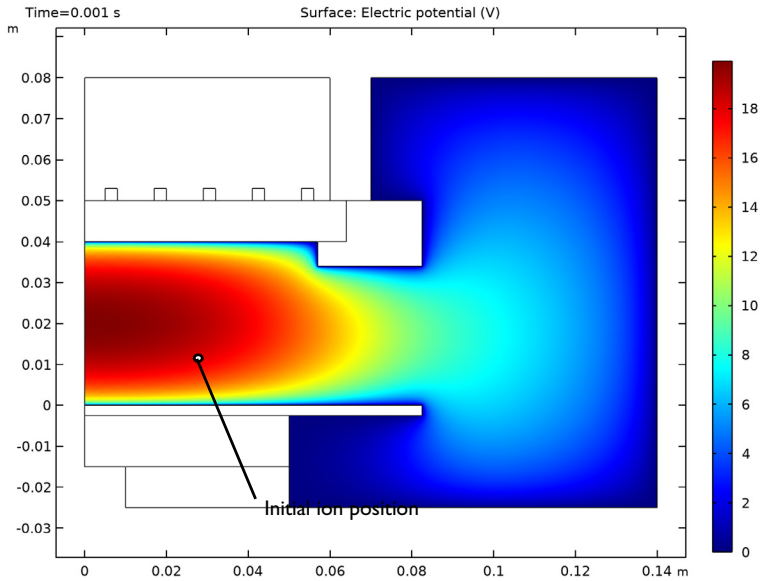

Figure 1: Plot of the plasma potential used to compute the IEDF.

The IEDF is plotted in Figure 2. Most of the ions have kinetic energy between around 20 and 22 eV. At the initial starting coordinate, the plasma potential is 20.98 V, so it is expected that the kinetic energy of the ions at the wall is of similar order. As the pressure decreases the collision frequency between ions and neutrals is reduced, so the IEDF should shift to the right, toward the maximum value given by the plasma potential. As the pressure increases the sheath becomes more collisional which inhibits the ions from reaching higher

energies. Of course, changing the pressure results in a change in the discharge characteristics which may alter the shape and magnitude of the IEDF in a nonlinear way.

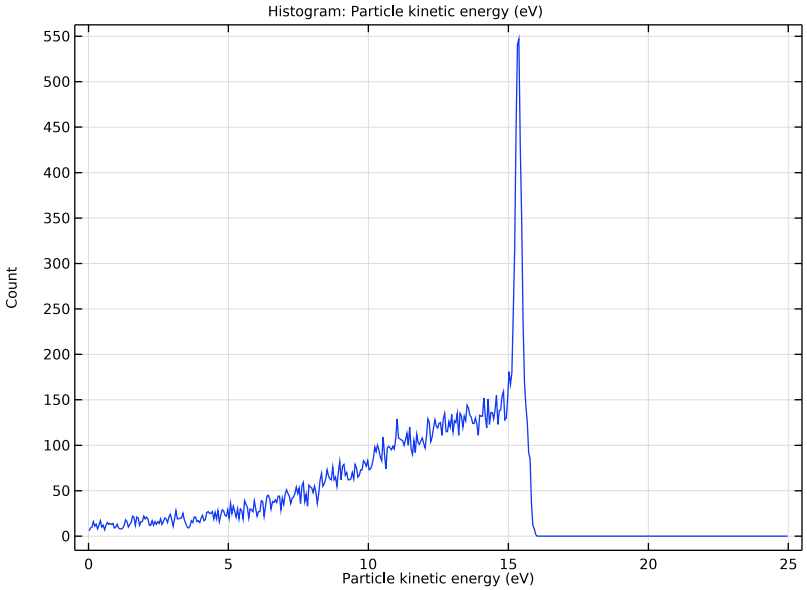

Figure 2: Plot of the ion energy distribution function (IEDF) in an inductively coupled plasma.

The angle at which the ions are striking the wafer surface are plotted in Figure 3. Due to the fact that the ions are released relatively close to the wafer surface, the range of angles is small, typically between -20 and 20 degrees. The plot is not quite symmetric due to the presence of a small outward component of the ambipolar electric field.

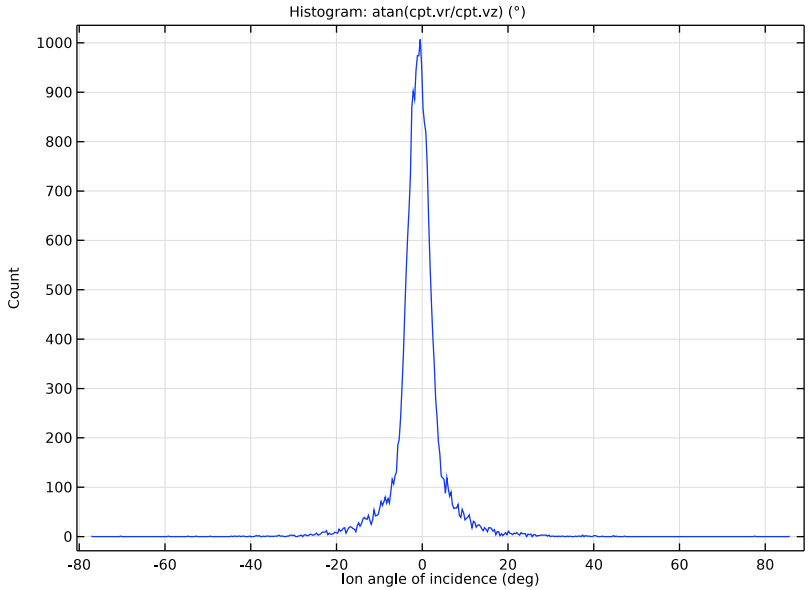

Figure 3: Plot of the angle at which the ions strike the surface of the wafer.

The ion angular energy distribution function is plotted in Figure 4. The angle is not quite symmetric about zero due to the profile of the electric field at the release point.

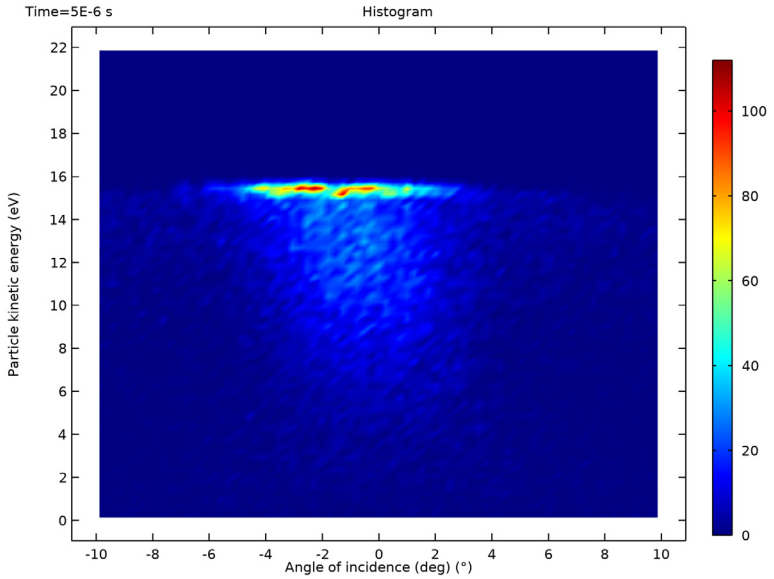

Figure 4: Plot of the ion angular energy distribution function.

Notes About the COMSOL Implementation

This model is most conveniently solved by opening an existing model in the Plasma Module Application Library, then computing the ion trajectories.

References

1. O.V. Vozniy, G.Y. Yeom, and A. Yu. Kropotov, "Plasma Potential Influence on Ion Energy Distribution Function in ICP Source", PSE, vol 5, no 1-2, pp. 28–33, http://www.pse.scpt.org.ua/en/jornal/1-2_07/3.pdf.

2. M. Surendra, "Radiofrequency Discharge Benchmark Model Comparison", *Plasma Sources Sci. Technol*, vol. 4, pp 56–73, 1995.

3. A. V. Phelps, "The application of scattering cross sections to ion flux models in discharge sheaths", *J. Appl. Phys.* vol. 76, pp. 747–753, 1994.

Application Library path: `Plasma_Module/Inductively_Coupled_Plasmas/ion_energy_distribution_function`

Modeling Instructions

Start by opening the model of the inductively coupled GEC reference cell from the **Plasma Module** Application Library.

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

Browse to the model's Application Libraries folder and double-click the file `argon_gec_icp.mph`.

COMPONENT 1 (COMP1)

Now add a **Charged Particle Tracing** interface to compute the ion energy distribution function.

1 From the **Home** menu, choose **Add Physics**.

ADD PHYSICS

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

2 In the tree, select **AC/DC>Particle Tracing>Charged Particle Tracing (cpt)**.

3 Click **Add to Component 1** in the window toolbar.

4 From the **Home** menu, choose **Add Physics**.

ROOT

From the **Home** menu, choose **Add Study**.

ADD STUDY

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

2 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Plasma (plas)** and **Magnetic Fields (mf)**.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 From the **Home** menu, choose **Add Study**.

CHARGED PARTICLE TRACING (CPT)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** node, then click **Charged Particle Tracing (cpt)**.

2 In the **Settings** window for **Charged Particle Tracing**, locate the **Domain Selection** section.

3 Click  **Clear Selection**.

4 Select Domain 3 only.

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
Mw	0.04[kg/mol]	0.04 kg/mol	Ion molecular weight
mi	Mw/N_A_const	6.6422E-26 kg	Ion mass

DEFINITIONS

Analytic 1 (an1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

Enter the analytic approximation for momentum cross section for elastic scattering between Ar+ ions and neutral Ar atoms, which depends on the kinetic energy of the particles.

2 In the **Settings** window for **Analytic**, type `Qm` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `1.15e-18*x^(-0.1)*(1+0.015/x)^0.6`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

Analytic 2 (an2)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

Enter the analytic approximation for isotropic elastic collision between Ar+ ions and neutral Ar atoms from, which depends on the kinetic energy of the particles.

2 In the **Settings** window for **Analytic**, type `Qi` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `2e-19/(x^(0.5)*(1+x))+3e-19*x/(1+x/3)^(2.3)`.

4 Locate the **Units** section. In the **Arguments** text field, type `eV`.

5 In the **Function** text field, type `m^2`.

CHARGED PARTICLE TRACING (CPT)

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Mass** section.

3 In the m_p text field, type `mi`.

4 Locate the **Charge Number** section. In the Z text field, type `1`.

Now add an **Electric Force** feature. The electric potential comes from the solved plasma model. Specify that piecewise polynomial recovery should be used when computing the electric force. This results in a more accurate reconstruction of the electric field.

Electric Force 1

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

2 Select Domain 3 only.

3 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

4 From the **Specify force using** list, choose **Electric potential**.

5 From the V list, choose **Electric potential (plas)**.

6 Locate the **Advanced Settings** section. Select the **Use piecewise polynomial recovery on field** check box.

Now you add the collisional force between the ions and background gas. The collision frequency is a function of the neutral number density (`plas.Nn`), the elastic and charge exchange cross section and the particle velocity (`cpt.V`).

Collisions 1

1 In the **Physics** toolbar, click **Domains** and choose **Collisions**.

2 Select Domain 3 only.

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

4 In the N_d text field, type `plas.Nn`.

5 In the M_g text field, type `Mw`.

6 In the T text field, type `plas.T`.

Elastic 1

1 In the **Physics** toolbar, click **Attributes** and choose **Elastic**.

2 In the **Settings** window for **Elastic**, locate the **Collision Frequency** section.

3 In the σ text field, type `Qi(cpt.Ep)`.

Collisions 1

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

Resonant Charge Exchange 1

1 In the **Physics** toolbar, click **Attributes** and choose **Resonant Charge Exchange**.

2 In the **Settings** window for **Resonant Charge Exchange**, locate the **Collision Frequency** section.

3 In the σ text field, type `(Qm(cpt.Ep)-Qi(cpt.Ep))/2`.

Release from Grid 1

1 In the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{r,0}$ text field, type `0.02`.

4 In the $q_{z,0}$ text field, type `0.005`.

5 Locate the **Initial Velocity** section. From the **Initial velocity** list, choose **Maxwellian**.

6 In the $N_{\mathbf{v}}$ text field, type `150`.

7 In the T_0 text field, type `400`.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2** 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 `range(0,5.0e-6/30,5.0e-6)`.

4 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

5 From the **Method** list, choose **Solution**.

6 From the **Study** list, choose **Study 1, Frequency-Transient**.

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

RESULTS

Ion Energy Distribution Function

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Ion Energy Distribution Function` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.
4. From the **Time selection** list, choose **Last**.

Histogram 1

1. Right-click **Ion Energy Distribution Function** and choose **Histogram**.
2. In the **Settings** window for **Histogram**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Charged Particle Tracing>Velocity and energy>cpt.Ep - Particle kinetic energy - J**.
3. Locate the **Expression** section. From the **Unit** list, choose **eV**.
4. Locate the **Bins** section. From the **Entry method** list, choose **Limits**.
5. In the **Limits** text field, type `range(0,25/500,25)`.
6. In the **Ion Energy Distribution Function** toolbar, click **Plot**.

Ion Angular Distribution Function

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Ion Angular Distribution Function` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.
4. From the **Time selection** list, choose **Last**.

Histogram 1

1. Right-click **Ion Angular Distribution Function** and choose **Histogram**.
2. In the **Settings** window for **Histogram**, locate the **Expression** section.
3. In the **Expression** text field, type `atan(cpt.vr/cpt.vz)`.
4. Locate the **Bins** section. In the **Number** text field, type `500`.
5. Locate the **Expression** section. From the **Unit** list, choose **°**.
6. In the **Ion Angular Distribution Function** toolbar, click **Plot**.

Ion Angular Distribution Function

1. In the **Model Builder** window, click **Ion Angular Distribution Function**.
2. In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `Ion angle of incidence (deg)`.

5 In the **Ion Angular Distribution Function** toolbar, click **Plot**.

Ion Angular Energy Distribution Function

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Ion Angular Energy Distribution Function` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.

4 From the **Time (s)** list, choose **5E-6**.

Histogram 1

1 In the **Ion Angular Energy Distribution Function** toolbar, click **More Plots** and choose **Histogram**.

2 In the **Settings** window for **Histogram**, locate the **x-Expression** section.

3 In the **Expression** text field, type `atan(cpt.vr/cpt.vz)`.

4 From the **Unit** list, choose **°**.

5 Select the **Description** check box.

6 In the associated text field, type `Angle of incidence (deg)`.

7 Locate the **y-Expression** section. In the **Expression** text field, type `cpt.Ep`.

8 From the **Unit** list, choose **eV**.

9 Locate the **Bins** section. Find the **x bins** subsection. From the **Entry method** list, choose **Limits**.

10 In the **Limits** text field, type `range(-10,20/79,10)`.

11 Find the **y bins** subsection. From the **Entry method** list, choose **Limits**.

12 In the **Limits** text field, type `range(0,22/79,22)`.

Ion Angular Energy Distribution Function

1 In the **Model Builder** window, click **Ion Angular Energy Distribution Function**.

2 In the **Ion Angular Energy Distribution Function** toolbar, click **Plot**.

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