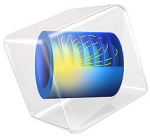

Pulsed Capacitively Coupled Plasma Discharge

Introduction

Pulsed plasma processing, or in more general terms, modulated-power plasma processing allows both the discharge chemistry to be altered, as well as the properties of the deposited films. The etch or deposition rate can also be maintained for lower input powers compared to continuous mode discharges.

Model Definition

A modulated, or pulsed discharge generally consists of 4 regimes which define the ***characteristic period*** of the discharge:

- Turn-on (sometimes known as ramp-up).
- On, or high power period.
- Turn-off (sometimes known as ramp-down).
- Off, or low power period.

These 4 operating conditions are then repeated billions of times over the course of a process. Thus, despite operating 4 different regimes within one characteristic period, the discharge can be considered to be time periodic within one characteristic period.

Computational Considerations

Particular care must be taken when using the Pulsed option in the Metal Contact feature. The Plasma, Time Periodic interface defines the characteristic period using an additional independent variable, which must be discretized in space using a mesh. In order to resolve the RF modulation within the on period, at least 30 mesh elements are required per RF period. Consider the case where the discharge is on for 10 cycles at 13.56 MHz (780 ns), then off for another 100 cycles (7.8 us). During the on-cycle, we need to use 30 mesh elements for each RF period (78 ns). During the off-cycle, there is no RF modulation, so we can use around 100 mesh elements for the entire 7.8 us. So, we need a total of 310 mesh elements to discretize the extra coordinate representing the characteristic period. This represents a 10 fold increase in computation demand compared to a continuous mode discharge, which would only require 30 mesh elements in the extra coordinate. Therefore, the pulsed option is very computationally expensive, and even 1D models are expected to take a significant amount of time to solve.

The Dual pulse option, where the off-period is replaced by a low power period is even more computationally expensive, since the low power period also needs 30 mesh elements per RF period. So, for the above example, where the 100 cycle off period is replaced by

low power operation, we would need 3000 mesh elements to resolve this part. This would make such a model 100 x more expensive than the same continuous mode discharge.

When considering using the pulsed discharge option, use the following to estimate the computation demand:

- In 1D, set up the model and chemistry of interest, and solve the problem using a continuously operated mode. The computation time for this is t_c
- For the Pulsed option, the expected computation time would be t_c multiplied by the number of RF periods than the discharge is on for.
- For the Dual pulsed option, the expected computation time would be t_c multiplied by the number of RF periods within the characteristic period.

Ion Transport

When using the Plasma, Time Periodic interface, the mass fraction of the heavy species, the ions and neutrals, can be computed in just the base geometry or in the product space spanning the base geometry and characteristic period coordinate. Solving for the ions in the base geometry only is much more efficient, and numerically stable, but it does assume that the number density and spatial distribution doesn't change over the characteristic period. This is a reasonable assumption for the continuous mode operation, but for pulsed discharges with long on or off periods, this assumption begins to break down. Therefore, for pulses where the characteristic period lasts for more than a few microseconds, it may become necessary to solve for the heavy species in the product space, which may be too computationally expensive, or impossible to obtain a converged solution. Therefore, the pulsed options can really only be used to study the electrical characteristics of a discharge, and not the transport of heavy species to reactor walls for discharges with prolonged off periods.

Results and Discussion

The I-V characteristics over the entire period are presented in Figure 1. As expected, the current is zero during nearly all of the off period, then ramps up to around 0.8 A. Interestingly, the current is asymmetric, the positive current peaks at 0.9 A, but on the negative side the current peak is -0.8 A. A close up of the I-V characteristics is presented in Figure 2, and indicates that the negative part of the current is increased compared to the positive part during the ramp up and ramp down. The total current when averaged over the entire period still remains zero.

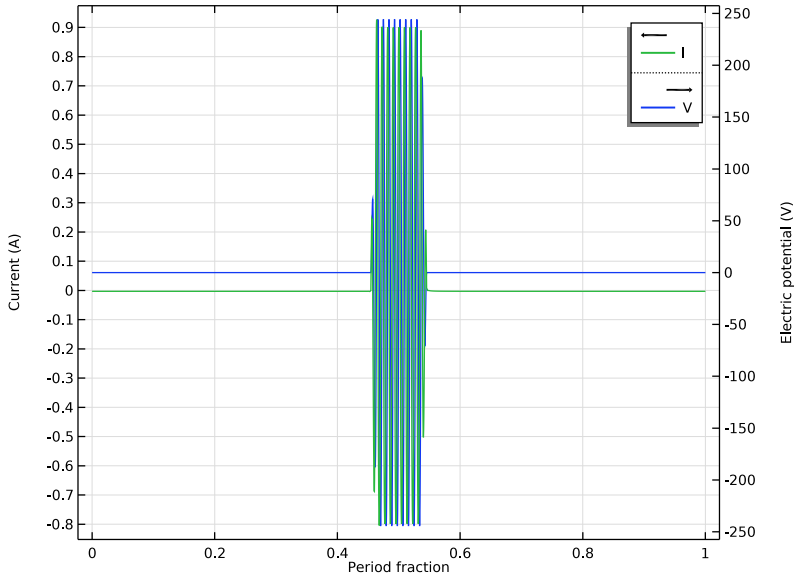

Figure 1: I-V characteristics over the entire period.

The electron density in the center of the reactor is shown in Figure 3. The electron density actually drops by more than 10 % during the excitation part of the period. The electron temperature, shown in Figure 4 shows the opposite behavior, it increases significantly during the electrical excitation, then begins to decay when the power is off. Finally, the electric potential in the center of the reactor is shown in Figure 5. The potential always remains positive with respect to the walls, and shows typical behavior when the power is on. When the power is off, the electric potential decays from 70 V to 45 V by the time that the power comes back on.

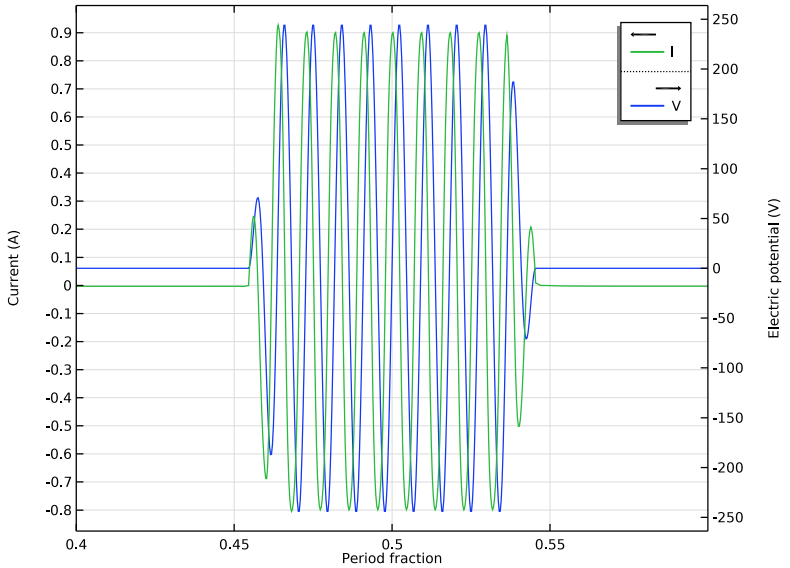

Figure 2: Close up of the I-V characteristics when the pulse is turned on.

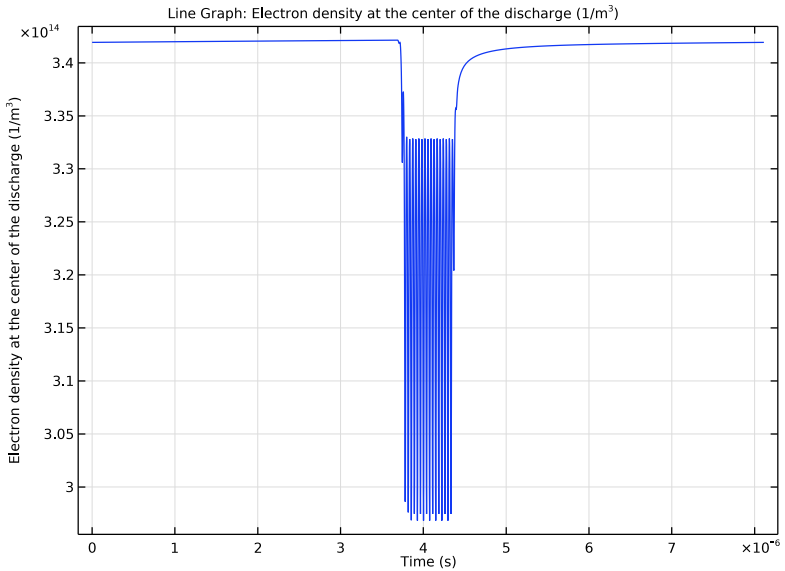

Figure 3: Plot of the electron density in the center of the reactor vs. time over the entire period.

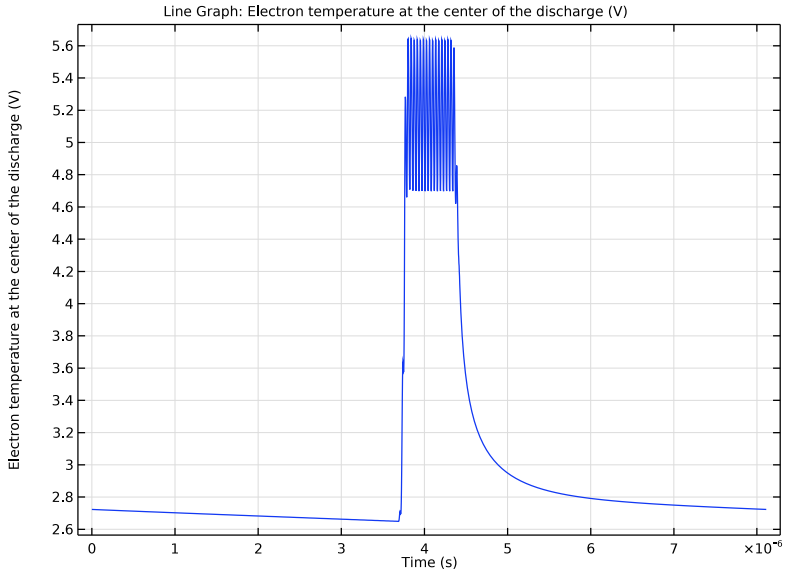

Figure 4: Plot of the electron temperature in the center of the reactor vs. time.

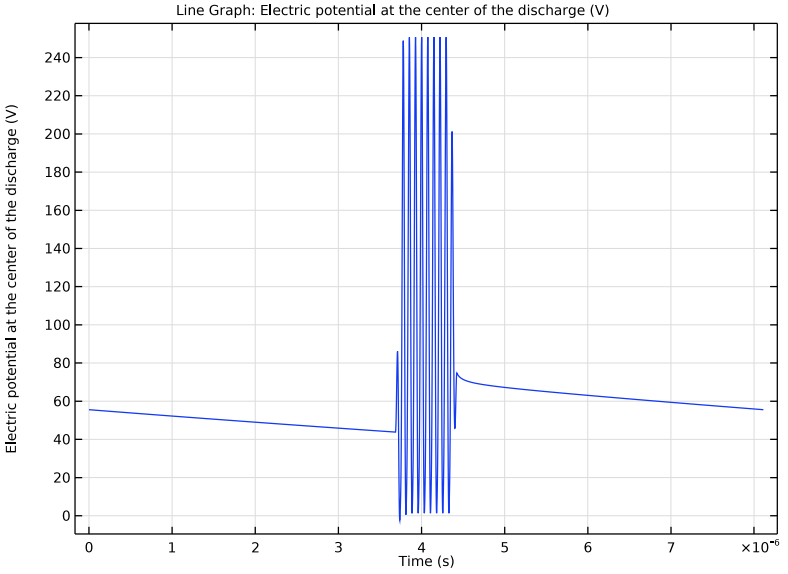

Figure 5: Plot of the electric potential in the center of the reactor vs. time over the entire period.

Reference

1. M.A. Lieberman and A.J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, John Wiley & Sons, 2005.

Application Library path: `Plasma_Module/Capacitively_Coupled_Plasmas/pulsed_ccp_discharge`

Modeling Instructions

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

NEW

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

Select the **Plasma, Time Periodic (ptp)** interface and the **Time Periodic** study to compute the periodic steady state solution of the pulsed discharge.

MODEL WIZARD

1. In the **Model Wizard** window, click **1D**.
2. In the **Select Physics** tree, select **Plasma>Plasma, Time Periodic (ptp)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Periodic**.
6. Click **Done**.

Add some parameters to facilitate the setup of the model.

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
f0	13.56[MHz]	1.356E7 Hz	Base frequency
As	0.25*pi*(0.3[m])^2	0.070686 m²	Wafer surface area
p0	0.1[torr]	13.332 Pa	Pressure
T0	300[K]	300 K	Temperature
Prf	1[W]	1 W	Single pulse power
Non	10	10	Number of periods the pulse is on
Noff	100	100	Number of periods the pulse is off
Nrampup	1	1	Number of cycles to ramp to on state
Nrampdown	1	1	Number of cycles to ramp to off state
Nelon	30	30	Number of elements per period for the on period
Neloff	100	100	Number of elements for the off period
Ncycles	Non+Noff	110	Total number of cycles
period_single	Ncycles/f0	8.1121E-6 s	Total period

The geometry is very simple and involves a discharge gap of 2.5cm.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
0.025

Import cross section data for Argon which automatically adds the electron impact reactions and species to the model.

PLASMA, TIME PERIODIC (PTP)

Cross Section Import 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Plasma, Time Periodic (ptp)** and choose **Cross Section Import**.

2 In the **Settings** window for **Cross Section Import**, locate the **Cross Section Import** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `Ar_xsecs.txt`.

Reaction 1

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

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ars+Ars=>e+Ar+Ar+`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `3.734E8`.

7: Ars+Ars=>e+Ar+Ar+

1 Right-click **Reaction 1** and choose **Duplicate**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ar+Ars=>Ar+Ar`.

4 Locate the **Reaction Parameters** section. In the k^{f} text field, type `1807`.

Select that the ground state Argon is the species to come from the mass constraint.

Species: Ar

1 In the **Model Builder** window, click **Species: Ar**.

2 In the **Settings** window for **Species**, locate the **Species Formula** section.

3 Select the **From mass constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **Ar**.

Species: Ars

1 In the **Model Builder** window, click **Species: Ars**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Ar**.

For positive Argon ions, use the local field approximation for the temperature and field dependent mobility.

Species: Ar+

1 In the **Model Builder** window, click **Species: Ar+**.

2 In the **Settings** window for **Species**, locate the **Species Formula** section.

3 Select the **Initial value from electroneutrality constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **Ar**.

5 Click to expand the **Mobility and Diffusivity Expressions** section. From the **Specification** list, choose **Specify mobility, compute diffusivity**.

6 From the **Ion temperature** list, choose **Use local field approximation**.

7 Click to expand the **Mobility Specification** section. From the **Specify using** list, choose **Argon ion in argon**.

Plasma Model 1

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

2 In the **Settings** window for **Plasma Model**, locate the **Model Inputs** section.

3 In the T text field, type `T0`.

4 In the p_A text field, type `p0`.

For the surface reactions, only the ions contribute to secondary electron emission.

Surface Reaction 1

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

2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ar+=>Ar`.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `0`.

Surface Reaction 2

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

2 In the **Settings** window for **Surface Reaction**, locate the **Boundary Selection** section.

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

4 Locate the **Reaction Formula** section. In the **Formula** text field, type `Ars=>Ar`.

5 Locate the **Secondary Emission Parameters** section. In the γ_i text field, type `0`.

6 In the ε_i text field, type `0`.

Wall 1

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

2 In the **Settings** window for **Wall**, locate the **Boundary Selection** section.

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

Ground 1

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

2 Select Boundary 2 only.

Now set the characteristics for the pulse. If the **Equation** section is expanded, an image is shown to make it easier to set the pulse settings.

Metal Contact 1

1 In the **Physics** toolbar, click → **Boundaries** and choose **Metal Contact**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 From the **Source** list, choose **RF**.

5 Locate the **RF Source** section. From the **Periodic function** list, choose **Pulsed**.

6 In the P_{rf} text field, type `Prf`.

7 In the f_p text field, type `f0`.

8 Select the **Create a mesh suggestion for the extra dimension** check box.

9 In the N_{on} text field, type `Non`.

10 In the N_{off} text field, type `Noff`.

11 In the $N_{\mathrm{low,high}}$ text field, type `Nrampup`.

12 In the $N_{\mathrm{high,low}}$ text field, type `Nrampdown`.

13 In the $N_{\mathrm{elp,on}}$ text field, type `Nelon`.

14 In the $N_{\mathrm{el,off}}$ text field, type `Neloff`.

Solve for the heavy species in the base geometry only. This is more stable than solving for them in the product space, but it does assume that the ion density does not change over the period. For pulses with a long off period, this might not be an appropriate assumption.

15 In the **Model Builder** window, click **Plasma, Time Periodic (ptp)**.

16 In the **Settings** window for **Plasma, Time Periodic**, locate the **Out-of-Plane Thickness** section.

17 In the A text field, type `As`.

18 Locate the **Extra Dimension Settings** section. In the P_{xd} text field, type `period_single`.

19 From the **Mesh specification** list, choose **Metal Contact 1**.

20 From the **Heavy species selection** list, choose **Base geometry**.

Use a mesh that is finer close to the walls, where the sheath region is expected.

MESH 1

Edge 1

In the **Mesh** toolbar, click  **Edge**.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `75`.

5 In the **Element ratio** text field, type `5`.

6 Select the **Symmetric distribution** check box.

7 Click  **Build All**.

SINGLE PULSE

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

2 In the **Settings** window for **Study**, type `Single Pulse` in the **Label** text field.

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

The default plot of current and voltage over the period makes visualization of the I-V characteristics difficult, so set some manual axis limits.

RESULTS

Current and Voltage, Metal Contact 1 (ptp)

1 In the **Model Builder** window, under **Results** click **Current and Voltage, Metal Contact 1 (ptp)**.

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

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0.4`.

5 In the **x maximum** text field, type `0.6`.

6 In the **Current and Voltage, Metal Contact 1 (ptp)** toolbar, click **Plot**.

We now want to plot the electron density, temperature and plasma potential at the center of the discharge. We can do this without having to add a **Time Periodic to Time Dependent** study if we make use of the `atxd()` operator.

Electron Density vs. Time

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

2 In the **Settings** window for **1D Plot Group**, type `Electron Density vs. Time` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Single Pulse/Solution 1 (2) (sol1)**.

Now add the line graph. The syntax `comp1.atxd1(0.0125,ptp.ne)` means that we visualize the expression for the electron density `ptp.ne` at the center of the reactor, corresponding to the position `x=0.0125`.

Line Graph 1

1 Right-click **Electron Density vs. Time** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `comp1.atxd1(0.0125, ptp.ne)`.

5 Select the **Description** check box.

6 In the associated text field, type `Electron density at the center of the discharge`.

Now change the definition of the x-axis to time by multiplying the space coordinate in the extra dimension by the total time for the period.

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

8 In the **Expression** text field, type `x1_ptp[1/m]*period_single`.

9 In the **Electron Density vs. Time** toolbar, click **Plot**.

10 Select the **Description** check box.

11 In the associated text field, type `Time`.

12 In the **Electron Density vs. Time** toolbar, click **Plot**.

Use the same technique as above to make plots for the electron temperature and plasma potential.

Electron Temperature vs. Time

1 In the **Model Builder** window, right-click **Electron Density vs. Time** and choose **Duplicate**.

2 In the **Model Builder** window, click **Electron Density vs. Time 1**.

3 In the **Settings** window for **1D Plot Group**, type `Electron Temperature vs. Time` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `comp1.atxd1(0.0125,ptp.Te)`.

4 In the **Description** text field, type `Electron temperature at the center of the discharge`.

5 In the **Electron Temperature vs. Time** toolbar, click  **Plot**.

Electric Potential vs. Time

1 In the **Model Builder** window, right-click **Electron Temperature vs. Time** and choose **Duplicate**.

2 In the **Model Builder** window, click **Electron Temperature vs. Time 1**.

3 In the **Settings** window for **1D Plot Group**, type `Electric Potential vs. Time` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `comp1.atxd1(0.0125,ptp.V)`.

4 In the **Description** text field, type `Electric potential at the center of the discharge`.

5 In the **Electric Potential vs. Time** toolbar, click  **Plot**.