1 Sheath Model

1.1 Introduction

When plasmas with quasi-neutrality ($n_e \approx n_i$) are joined to wall surfaces, a positively charged layer called *sheath* is required in physics to maintain the balance of electrons and ions. The electron thermal velcocity $(eT_e/m_e)^{1/2}$ is at least 100 times the ion thermal velocity $(eT_i/m_i)^{1/2}$, as $T_e \geq T_i$ and $m_e \ll m_i$. Let us assume an initial plasma with zero electric potenital and E-field everywhere, since $n_e = n_i$at $t = 0$. The electrons are not confined by any field or potential and hence move faster to the walls than ions. On a short timescale, some electrons near the walls are lost, leading to net positive space charges near the walls. This positively charged space, which is SHEATH, creates an E-field pointing to the walls, reducing the electron speed and increasing the ion speed to the walls. Eventually, the loss of electrons and ions balance each other and plasma remains quasi-neutral. Sheath plays an important role in the plasma etching. As positive ions flowing out of the bulk plasma enter the sheath, they get accelerated by the sheath fields and pick up high energies as they traverse across the sheath. The ions carry these high energies and delivers to the materials surface, such as Si surface. The ion etch rates, selectivity and damage are also impacted by the energies, which are determiend by the sheath. A diagram of sheath can be seen in the figure below.

Within the Langmuir model, Sheath model serves as a connector between Reactor model and Feature model. It takes the E-filed and species from the Reactor model and compute the angular and energy distribution of electrons and ions, which is fed into the Feature model as input. Sheath model uses particle tracing algorithm and basically traces particles under varying E-field. Particle collisions are taken into account and they widen the distribution of angle. In the code structure, modules from Feature model, such as particle and move, can be shared with Sheath model.

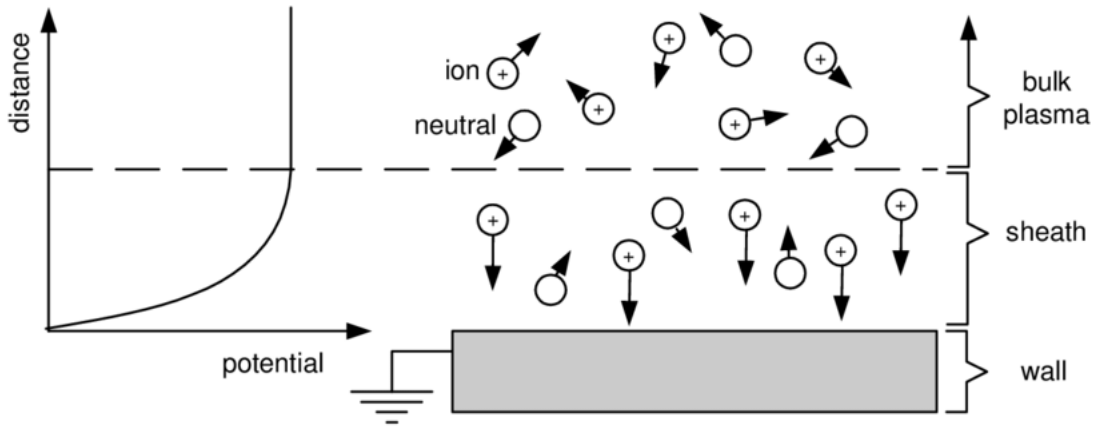

Figure 1: The plasma sheath. Ions in the plasma happen upon the sheath, where they are accelerated to the wall. At the wall, ions are neutralized by electrons from the ground and return to the bulk.

1.2 Collisionless Sheath

1.2.1 What is collisionless sheath

When the ion mean free path is much larger than the sheath thinkness, the sheath is called a collisionless sheath. Within a collisionless sheath, the velocites of ions are only determined by the sheath field and ions are continuously accelerated by the sheath field. Ions pick up energies as they enter the plasma-sheath edge and exit the sheath with an energy distribution of a bimodal shape, seen the figure below. At low frequencies ($\tau_{ion}/\tau_{rf} \ll 1$, transverse time of ion is much smaller than the RF period), the ions traverse the sheath within a small fraction of an RF cycle. The phase of the RF cycle at which ions enter the sheath determines their energies at the exit. In this case, the IED (Ion Energy Distribution) is broad and bimodal, with the two peaks corresponding to the minimum and maximum of the sheath drops. At high frequency ($\tau_{ion}/\tau_{rf} \gg 1$, transverse time of ion is much larger than the RF period), it takes the ions many RF cycles to cross the sheath. In such a scenario, the net energy gained by the ions is determined by the DC component, which is the time-averaged sheath voltage. The effect of phase at which they enter the sheath is significantly reduced. The IED is still bimodal, but much narrower.

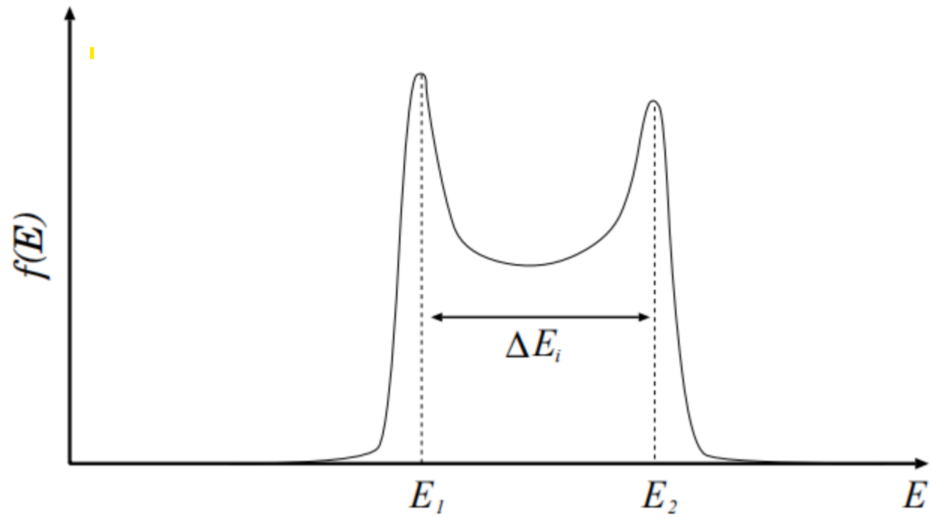

Figure 2: A bimodal ion energy distribution.

1.2.2 Analytic Collisionless Sheath Model

Benoit-Cattin et al[] obtained an analytic solution for IED at the high-frequency regime ($\tau_{ion}/\tau_{rf} \gg 1$, transverse time of ion is much larger than the RF period), assuming

1. a constant sheath thickness, $\bar{s}$
2. a uniform sheath electric field, $\vec{E}$is independent of position x
3. a sinusoidal sheath voltage $V_{sh}(t) = V_{dc} + V_s sin(\omega t)$
4. zero initial ion velocity at the plasma-sheath boundary, $v_{ion}(x = \bar{s}) = 0$

The resulting expressions for $\Delta E_i$and the IED are

$$\Delta E_i = \frac{2eV_s}{\bar{s}\omega}(\frac{2eV_{dc}}{m_i})^{1/2} = \frac{3eV_s}{\pi}(\frac{\tau_{rf}}{\tau_{ion}})$$

$$f(E) = \frac{dn}{dE} = \frac{2n_t}{\omega \Delta E_i}[1 - \frac{4}{\Delta E_i^2}(E - eV_{dc})^2]^{-1/2}$$

where $n_t$is the number of ions entering the sheath per unit time.

The calculations yield a bimodal IED with two peaks symmetric about $eV_{dc}$and ΔE_iproportional to $\frac{\tau_{rf}}{\tau_{ion}}$, seen the figure below.

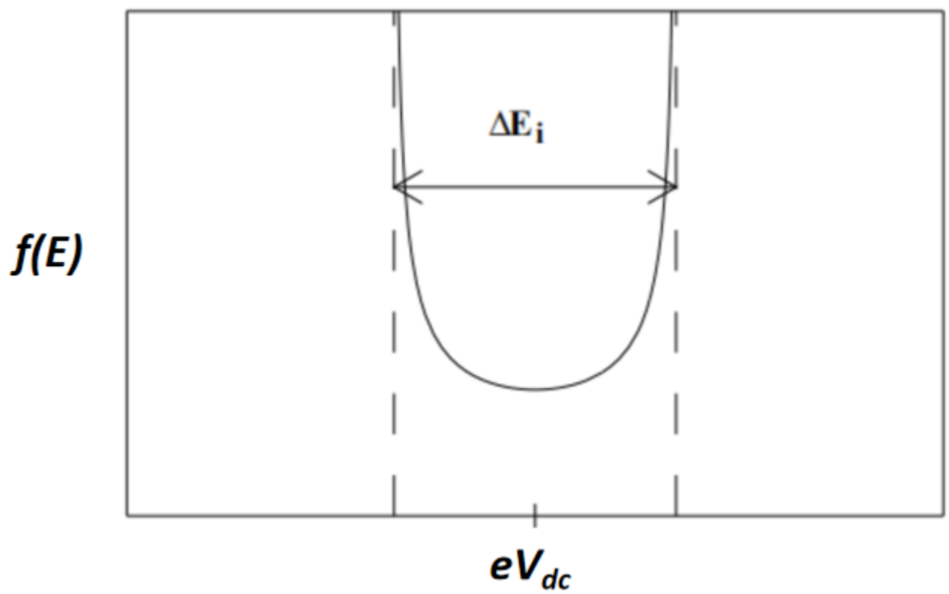

Figure 3: The plot of analytic solution for IED at the regime of high frequency $(\tau_{ion}/\tau_{rf} \gg 1)$. The singular peaks are due to the assumption of a mono-energetic initial ion velocity distribution.

1.2.3 Collisionless Sheath Model

In the collisionless sheath model, we only need to solve the Newton's euqation,

$$\frac{d}{dt}\vec{x} = \vec{v}$$

$$\frac{d}{dt}\vec{v} = \frac{eq}{m_i}\vec{E}(t)$$

$$\vec{E}(\vec{x}, t) = f(V_{sh}(x, t), s(t))$$

$$\vec{x}, \vec{v} - position, velocity$$

$$e - elementary\, charge$$

$$q - \#\, of\, charges\, carried\, by\, ion$$

$$\vec{E}(\vec{x}, t) - electric\, field\, within\, sheath$$

$$V_{sh}(\vec{x},t) - sheath\,potential$$

$$s(t) - sheath\,thickness$$

1.3 Collisional Sheath

When the mean free path of ions, λ_{ion}, is much smaller than the sheath thickness, the ions entering the sheath will experience collisions before exit. Collisions can alter the velocity, both speed and angle. Since the ion density is much smaller than background neutral density within the sheath, ion-neutral collisions dominate the ion collisions. In the sheath model, there is no ion-ion collisions, or even interactions. In another word, ions are independent from each other. The probability of a collision event occurring depends on the ion-neutral collision frequency, v_{in}, which is defined as:

$$v_{in} = N_d \sigma |\vec{v}_i - \vec{v}_g|$$

$$N_d - backgroud\,number\,density\;(m^{-3})$$

$$\sigma - ion - neutral\,charge\,exchange\,collision\,cross\,section\;(m^2)$$

$$\vec{v}_i, \vec{v}_g - ion\,velocity,\,background\,gas\,velocity\;(m/s)$$

The collision probability defined as

$$P = 1 - exp(-v_{in}\Delta t) = 1 - exp(-\frac{\Delta x}{\lambda_{ion}})$$

If a collision occurs, the particle velocity is updated according to following expression:

$$\vec{v}_i^{'} = \frac{m_i\vec{v}_i + m_g\vec{v}_g - m_g|\vec{v}_i - \vec{v}_g|\vec{U}}{m_i + m_g}$$

$$\vec{v}_i^{'} - after - collision\,ion\,velocity$$

$$m_i, m_g - mass\,of\,ion,\,background\,gas$$

$$\vec{U} - a\,uniformly\,distributed\,random\,unit\,vector$$

in the equation above, $\vec{v}_g$ is sampled from a Maxwellian distribution function, assuming the background neutral gas is in thermal equilibrium state.

1.4 Analytic Sheath Model