Modeling Of Energy-Band Diagram for Plasma-Metal Junction

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Abstract. Plasma based technologies find wide technological applications. The theory for electrical properties of plasma is well established, for different systems including simple dc discharges to complex fusion machines, using fluid model and statistical model. However, there are still several areas that are unexplored and one of such topics is plasma-material interaction. In present investigation we propose the concept of energy band diagram for plasma-metal junction analogous to the energy band diagram of P-N junction. The I-V characteristics of P-N junction diode and Schottky barrier diode are explained using well established energy band theory. In this work the concept of energy-band diagram for plasma-metal junction has been introduced and concentrates on how the I-V characteristics of plasma-metal junction vary for metals with different work functions. Using the proposed energy band diagram, I-V characteristics of plasma-metal junction obtained numerically. The I-V characteristics obtained using this concept of energy-band diagram of plasma-metal junction is consistent with theory and therefore this concept may have wide impact on laboratory plasmas and may provide a new method for higher accuracy for experimental measurements.

1. Introduction

Semiconductor physics has reached advanced stage and contributed significantly in development of all areas of engineering and technology in last five decades. The basic principle of semiconductor physics is the energy band theory, which explains the differences in the electrical properties between metals, insulators and semiconductors [1]. The basic idea in the formation of energy bands is that the discrete energy levels of electrons split into a range of energy levels with a slightly different energies, called band, when atoms are brought together to form crystal[1,2]. This theory also talks about valence band and conduction band separated by a forbidden energy gap, which can be explained by the Quantum mechanical wave function for electron in periodic lattice. The most important part of conduction is related to how effectively the electrons can be transferred from valence band to conduction band [2].
Fermi level, is yet another parameter in the Energy band theory, which is the highest energy level filled at absolute zero.

Band diagram is a simplified representation of changes in band structure relative to Fermi level [1]. Another important aspect we study for a semiconductor material is its I-V characteristics, which can be used to analyse its electrical properties.

Being aware of this fact, we try to extend the same idea to the system of Plasma-Metal junction. Plasma is a quasi-neutral gas consisting of charged particles, which exhibit a collective behaviour[4]. Metal probes are inserted directly into plasma and the current collected by the probe for different voltages applied, can be easily monitored. Once, we obtain the I-V characteristics, important plasma parameters such as electron temperature, electron density, etc can be determined. Till date, this was done using much complicated probe theory. Probe method was introduced by Langmuir that does the direct measurement of plasma parameters such as electron density, electron temperature, etc. In this method, a probe is introduced at some point of plasma and various potentials are applied to it. This method is simple in terms of the equipment and the experimental setup. The complexity lies in the theory used for the analysis of probe data. The validity of this theory is limited to rarefied gases as well as magnetic field-free setups. The theory comprises of lengthy mathematical calculations including distribution functions and multiple integrals. Subsequently this technique was modified to design double probe, which worked without the aid of any reference electrodes. In this work, a theoretical model of energy band diagram is proposed and a numerical plot of I-V characteristics is obtained for three values of work function. In this way, we are trying to extend semiconductor theory to plasma-metal junction.

II. Energy Band Diagram

2.1. Energy band diagram of a PN junction

When P and N regions are diffused together to form a junction, then the forces acting on the charge carriers is summed up in the following figure.

![Schematic diagram of nature of forces acting in different regions of a P-N junction diode](image)

Figure 1. Schematic diagram of nature of forces acting in different regions of a P-N junction diode [1].

Initially, the majority charge carriers flow across the junction due to the force of diffusion from either side. Subsequently, the junction becomes deprived of free charge carriers. The junction will now be
comprised of immobile ions; with positive ions constituting the junction in N-side and negative ions constituting the junction in the P side. This charge separation leads to the development of an electric field which exerts a force on the charge carriers opposite to the direction of force of diffusion [1]. At thermal equilibrium, the flow of charge carriers stop as the force of diffusion experienced by the charge carriers is cancelled by the force exerted by the electric field developed in the junction and the charge flow stops [1, 2]. A potential barrier is developed across the junction owing to junction formation. The energy band diagram representing the thermal equilibrium condition of a PN junction is shown in Fig. 2.

When a PN junction is forward biased, the majority carriers in each side receives enough energy to cross the potential barrier and thus charges flow across the PN junction. A reverse biased PN junction leads to an increase in the potential barrier and thus no forward current appears across the junction. However, a small reverse current due to the presence of the minority carriers on each side of the PN junction arises. This is termed as reverse saturation current [2]. Mathematically, the behaviour of PN junction as described by William Shockley can be stated as [3]

\[ I = I_S \left( \frac{eV_a}{e \pi K T} - 1 \right) \]

Where, \( I \) is the diode current; \( I_S \) is the reverse saturation current; \( V_a \) is the applied voltage; \( e \) is the electronic charge; \( n \) is the quality factor (1 for ideal case; we consider ideal case here); \( K \) is the Boltzmann constant; \( T \) is the temperature in Kelvin. Clearly, when a diode is reverse biased, \( V_a \) is negative and \( eV_a \) starts falling and becomes small in magnitude. It can easily be neglected for high negative values of \( V_a \). The diode current is thus \( I \sim -I_S \) (reverse saturation current). The equation explains both forward and reverse bias characteristics of a diode effectively. The breakdown region is excluded from this equation.

2.2 Proposed Energy band diagram of a plasma-metal junction

Plasma consists of electrons, ions and neutrals which are free to roam around [5]. Thus, we can say that the behaviour of electrons in plasma will be similar to the behaviour of electrons in a free system. This means that the Fermi energy of the system is positive. i.e \( E_F > 0 \) [10]. Whereas metal is a bound system. Fermi level lies below vacuum level for a metal i.e \( E_F < 0 \). To start with, we assume Fermi energy of plasma to be fixed at Plasma potential. Plasma potential is even throughout the system for
uniform homogeneous plasmas and it is the highest potential that an electron can possess [5,9]. This validates our assumption of fixing the Fermi level at Plasma potential.

Figure 3 shows the energy band diagram of metal & plasma before formation of junction. In the strong non-equilibrium plasma condition, the spread of velocity distribution is narrow and can be assumed that electrons in the plasma will have energy between 0 V to $V_P$ V. The energy difference between the top of the electron sea in plasma to the vacuum level can also be called plasma potential. This is the potential possessed by plasma with respect to a grounded electrode. $E_F$ of electrons in a grounded electrons is lower than $E_F$ of electrons in plasma.

Figure 4 shows the energy band diagram for metal- plasma junction. After formation of junction, the electrons from plasma will move towards the metal, where lower energy states are available when compared to plasma. At thermal equilibrium, plasma will become positively charged and metal will become negatively charged and the band will bend in the direction opposite to the electric field. A potential is developed by virtue of it and the height of this potential is called sheath potential ($V_{sh}$) which is also called built-in potential. The sheath is formed around the metal [5, 6] which can be considered analogous to the metallurgical junction formed in a PN junction. It will be an uphill potential seen by electrons in plasma which prohibit the further flow of electrons to metal. At the same time, it will be downhill potential for ions where they accelerate and finally dump their energy on metal and causes secondary electron emission. For secondary electrons emitted from metal, this potential will be a downhill potential and causes ionization by collision with neutral. For a floating metal the value of $V_{sh}$ will be equal to $V_P - V_f$. For grounded metal this will be equal to $V_P$. The width of the sheath depends on the ratio of electron and ion mass, pressure and number of secondary electron emission from metal.
The non-neutral region between metal and plasma is known as sheath where the quasineutrality of plasma is broken. In this region, the electron density falls as we move towards the metal [7]. When a probe is inserted into plasma, it introduces a perturbation nearer to it. The potential of the probe with respect to plasma is called probe potential/biasing potential \( V_B \) [5]. The total current \( I \) in the external circuit is the sum of ion and electron current reaching the probe from plasma. This total current \( I \) as a function of \( V_B \) can be expressed as follows [8, 6]

\[
I = I_{es} e^{\left(\frac{e(V_p-V_B)}{kT}\right)} - I_{ls}, \text{for } V_B < V_p
\]

\[
I = -I_{ls} e^{\left(\frac{e(V_p-V_B)}{kT}\right)} + I_{es}, \text{for } V_B > V_p
\]

\[
I = I_{es} - I_{ls}, \text{for } V_B = V_p
\]

We incorporated the effect of work function in the expression for current collected and thus, (2), (3) and (4) was modified as follows[12]

\[
I = -I_{ls} e^{\left(\frac{e(V_p-V_B+\phi_m)}{kT}\right)} + I_{es}, \text{for } V_B > V_p
\]

\[
I = I_{es} e^{\left(\frac{e(V_p-V_B+\phi_m)}{kT}\right)} - I_{ls}, \text{for } V_B < V_p
\]

\[
I = I_{es} e^{\phi_m} - I_{ls} e^{-\phi_m}, \text{for } V_B = V_p
\]

When \( V_B > V_p \); the exponential term is diminished; the current is predominantly electronic saturation current. When \( V_B < V_p \); the electronic current falls exponentially with decrease in \( V_B \) and the ionic current comes into picture. When the probe potential is sufficiently negative, then all the excess electrons arriving at the probe are repelled and the electronic current influx practically equals the ionic current influx, leading to zero net current. The potential at which no net current is collected by the probe is called the floating potential \( V_f \) [6]. It is clear from the expression for PN junction current and current collected by the probe that they have a similar kind of exponential dependence with the applied/biasing voltage.
2.2.1 Numerical plot of I-V characteristics of plasma-metal junction

Equation (4), (5) and (6) highlights the relation between current and voltage across a plasma-metal junction. But the amount of current collected by a metal also depends on work function of a metal, which shows how effectively an electron can be transported from Fermi level to vacuum level. For identical plasma conditions the $I-V$ characteristics of three different metals having different work function of 4 eV, 5 eV, 6 eV are plotted in Fig. 5.

![I-V characteristics of plasma-metal junction for metals with different work functions](image)

Figure 5. Numerical plot of $I-V$ characteristics for plasma-metal junction for 3 metals having different work function.

The reason for the difference in $I-V$ characteristics for three metals having different work function can be explained as follows. In the region $V_B > V_P$, the dominant current component is electronic current whereas in the region $V_B < V_P$, it is ionic. When the probe bias is zero, the sheath potential will be equal to $V_P - \phi_m$. The field due to this potential difference will be a retarding field for electrons which are coming from plasma to metal surface and it will be a attracting force for ions. For metals which are having work function in the order $\phi_1 < \phi_2 < \phi_3$; the magnitude of electric field experience by ions and electrons will be in the order of $E_1 < E_2 < E_3$. Due to this decelerating electric field, the magnitude of electronic current collected by the metal in the region $V_B > V_P$ follow the order $I_1 > I_2 > I_3$. In the similar way ions in the plasma, face accelerating field in the order $E_1 < E_2 < E_3$. Due to this field, the magnitude of ionic current collected by the probe in the region $V_B < V_P$ will follow the order $I_1 < I_2 < I_3$. Also, qualitatively, for a metal with lower work function, more electronic current is collected. Thus, to stop the flow of electrons towards metal, more negative potential must be applied to the metal. Hence, the floating potential will be more negative for metal which has low work function, and the magnitude of floating potential decreases with the increase in work function. This is consistent with the plot we obtained. Thus, the theoretical plot obtained is consistent with the energy band diagram.

III. Conclusion
The study of the system of plasma-metal junction based on energy band theory simplifies its understanding. The theoretical plot of $I-V$ characteristics of a plasma-metal junction emphasize the fact that the magnitude of current collected by a metal probe depends on its work function. Further, this study implies that the magnitude of floating potential decreases with the increase in work function. In addition, it is observed from the plot that material having higher work function draws low electronic current in the forward bias. Similarly, in the reverse bias material having higher work function draws low ionic current. The plot of $I-V$ characteristics obtained for plasma-metal junction is consistent with its proposed energy band diagram. Thus, it is established that energy band diagram gives more accurate explanation of $I-V$ characteristics of metal-plasma junction and this may lead to new direction in applied plasma physics. Further, it paves a way for a better understanding of metal-plasma junctions in a simplified picture and we believe that this idea can be extended for various other plasma-metal junctions as well.

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