Ion Transport to a Photoresist Trench in a Radio Frequency Sheath

ZHANG Saiqian (张赛谦), DAI Zhongling (戴忠玲), WANG Younian (王友年)

School of Physics and Optoelectronic Technology, Dalian University of Technology, Dalian 116023, China

Abstract We present a model which is used to study ion transport in capacitively coupled plasma (CCP) discharge driven by a radio-frequency (rf) source for an etching process. The model combines a collisional sheath model with a trench model. The sheath model can calculate the ion energy distributions (IEDs) and ion angular distributions (IADs) to specify the initial conditions of the ions incident into the trench domain (a simulation area near and in the trench). Then, considering the charging effect on the photoresist sidewalls and the rf-bias applied to the substrate, the electric potentials in the trench domain are computed by solving the Laplace equation. Finally, the trajectories, IEDs and IADs of ions impacting on the bottom of the trench are obtained using the trench model. Numerical results show that as the pressure increases, ions tend to strike the trench bottom with smaller impact energies and larger incident angles due to the collision processes, and the existence of the trench has distinct influences on the shape of the IEDs and IADs. In addition, as the bias amplitude increases, heights of both peaks decrease and the IEDs spread to a higher energy region.

Keywords: ion motion, IED, IAD, charging effect, sheath, plasma etching, CCP

PACS: 52.40.Kh, 52.65.Cc, 52.77.Bn

DOI: 10.1088/1009-0630/14/11/03

1 Introduction

Plasma etching is one of the most important processes in the production of the semiconductor devices. Due to the quickly developing semiconductor industry, the scaling down of feature dimensions requires more precise control of the etching profile. IEDs and IADs of ions impacting onto the materials to be etched, together with the chemical and physical properties of the materials, have great influences on the etching anisotropic, etch yield, etch rate, etc. In semiconductor manufacture, ion transport in the local electric field near the material to be etched is a key to reduce profile deformations such as notching [1], sidewall bowing [2-3], and microtrenching [4]. In plasma etch processing, radio frequency capacitively coupled plasma (rf-CCP) is usually used to sustain the plasma and to accelerate the ions in the sheath due to its relatively simple structure and good uniformity [5]. Thus, the parameters of CCP discharge have significant influences on the characteristics of ions passing through the sheath, for example, the IEDs and IADs. Many models have been proposed to study the IEDs and IADs in CCPs [6-9]. A review of ion energy distributions in rf sheaths was made by KAWAMURA et al [6]. LEE et al. presented the pressure, voltage and frequency effects on IEDs using a particle-in-cell/Monte Carlo simulation [7]. To describe a collisional sheath in a dual-frequency CCP discharge plasma, DAI et al. proposed a self-consistent hybrid sheath model in a large range of frequencies [8]. In addition, the influence of fast neutrals is added by WANG et al. using a hybrid model [9]. Studies of ion behaviors influenced by the local electric field in and near the trench have been made to achieve a better understanding of the precise control of the etching profile [10-14]. ARNOLD and SAWIN studied the localized charging of a trench assuming an isotropic electron flux and monodirectional ion bombardment [10], but in practice, because of the collision processes in the sheath, ions have a distribution in incident angles rather than incident normal to the substrate. An entirely analytical physical model to explain charging damage with tracking the substrate potential was given by CHEUNG and CHANG [11]. KAMATA and ARIMOTO experimentally investigated the influence of the electron temperature and rf bias on charge build-up [12] in inductively coupled plasma (ICP). Recently, MADZIWA-NUSINOV et al. presented a self-consistent computation of the ion trajectories by considering the charging of the sidewalls [13]. It is noted that the model in Ref. [13] used a dc-bias voltage. However, an rf bias is widely used in etching processes. Therefore, it is necessary to study the ion transport with rf biases applied on electrodes. PALOV et al. studied the charging of submicron structures in a single and dual frequency capacitive rf discharge plasma [14], the IEDs were studied at different trench aspect ratios, but in their study a delta function was used to describe the initial ion in-

*supported by National Natural Science Foundation of China (Nos. 11075029, 10975030)
Zhang Saiqian et al.: Ion Transport to a Photoresist Trench in a Radio Frequency Sheath

cient energy. Therefore, for more consistent research, the IEDs obtained from a sheath model should be applied to specify the initial conditions of the incident ions.

In this paper, we use a combined model with a one dimensional (1D) sheath model and a two dimensional (2D) trench model. The sheath model is used to obtain the IEDs and IADs of the ions passing through the collisional sheath. In addition, the electric potential and ion transport in the trench domain are simulated using the 2D trench model. Finally by tracing ion trajectories near and in the trench, the IEDs and IADs at the sub-surface are found. The sheath and the trench models are described in the next section. Then in section 3, the numerical results and discussion are presented. Finally, the conclusion is given in section 4.

2 Model description

We consider a photoresist trench with a conductive bottom in the sheath region. A schematic diagram is shown in Fig. 1. Ions go through the sheath region and then enter the trench domain.

![Fig.1 Schematic diagram of the model and computational domain](image)

2.1 The sheath model

In the sheath region, a hybrid sheath model is applied which consists of a fluid method to describe the spatiotemporal evolution of the sheath and a Monte-Carlo method to describe the collision processes in the sheath. We can obtain the initial velocities and directions of ions entering the trench domain by sampling the distribution functions obtained from the sheath model. Because the thickness of the trench domain is thin compared to the sheath thickness, we can ignore the influences of the trench on the results of the sheath model.

For the one dimensional ion density \(n_i(x, t)\) and ion drift velocity \(u_i(x, t)\), they can be described by the cold ion fluid equations:

\[
\frac{\partial n_i}{\partial t} + \frac{\partial (n_i u_i)}{\partial x} = 0, \tag{1}
\]

\[
\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} = - \frac{e}{m_i} \frac{\partial V}{\partial x} - \nu u_i, \tag{2}
\]

where \(m_i\) is the ion mass, \(e\) is the elementary charge, \(V(x, t)\) is the electric potential and \(\nu = u_i N \sigma_i(u_i)\) is the total collision frequency for ions and neutrals, and here \(N\) is the neutral gas density, \(\sigma_i(u_i)\) is the total collision cross section.\(^{[15,16]}\)

The Poisson equation is also needed to form a closed equation set:

\[
\frac{\partial^2 V}{\partial x^2} = - \frac{e}{\varepsilon_0} (n_i - n_e), \tag{3}
\]

where \(\varepsilon_0\) is the permittivity of free space and \(n_e(x, t)\) is the electron density. Due to the electron plasma frequency \(\omega_{pe} = e^2 n_0 / \varepsilon_0 m_e\) being much higher than the rf frequency \(\omega\), we can assume that the electrons are inertialess and respond to the instantaneous electric field, thus the electron density satisfies the Boltzmann relation and we have

\[
n_e(x, t) = n_0 \exp \left( \frac{e V(x, t)}{k_B T_e} \right), \tag{4}
\]

where \(n_0\) is the plasma density, \(T_e\) is the electron temperature and \(k_B\) is the Boltzmann constant.

Eqs. (1)∼(4) coupled with the boundary conditions can be solved by numerical methods, so the electric potential, ion density distributions and so on can be obtained.

Then we describe the ion transport process in the sheath and use the Monte-Carlo methods to get the IEDs and IADs of ions passing through the sheath. The ion motion equation is used to determine the transport process of ions through the sheath:

\[
m_i \frac{d^2 x(t)}{dt^2} = e E(x, t), \tag{5}
\]

where \(m_i\) is the ion mass, and the electric field \(E(x, t)\) is determined by \(E(x, t) = - \frac{\partial V(x, t)}{\partial x}\) in the one dimension case.

For the collision processes, we consider the charge-exchange collisions and elastic collisions of ions with neutrals, the cross sections are relevant to the ion kinetic energy and shown as follows\(^{[15,16]}\):\(^{[15,16]}\):

\[
\sigma_{el} = 40.04(1.0 - 0.0563 \ln \varepsilon)^2, \tag{6}
\]

\[
\sigma_{cx} = 47.05(1.0 - 0.0557 \ln \varepsilon)^2, \tag{7}
\]

where \(\sigma_{cx}\) is the cross section for charge exchange collisions.

By using the Monte-Carlo methods, the occurrence of the collisions and the type of the collisions are determined by the stochastic sampling for the ion transport process in the sheath, and finally IEDs and IADs are obtained after ions go through the whole sheath region.
2.2 The trench model

Then we consider the ion transport behaviors in the trench domain. The simulation area is divided into square cells so that potentials can be applied to the nodes of the grid. As mentioned above, the thickness of the trench domain is small compared to the Debye length or the sheath thickness. So the initial velocities of ions entering the trench domain can be calculated from the IEDs obtained from the sheath model and the directions of their entry into the trench domain can be determined by sampling the angular distribution functions.

In the trench domain, as the dimensions of the photoresist mask are much smaller than the sheath thickness and electrode width, we ignore its influence on the potential at the upper boundary of the trench domain. Typically, the potential drop during the trench is smaller than 0.1 V [17], so here we assume that the potential at the upper boundary for the trench domain is equal to the potential at the electrode.

The photoresist is a block of dielectrics, so the floating potential at the surface of the photoresist can be found using Eqs. (8) and (9). Similarly, the potential of the trench domain is small compared to the Debye width, we ignore its influence on the potential at the surface of the photoresist. Last, we average the ion distributions over one rf cycle, so new boundary potentials on the surface of the photoresist can be found using Eqs. (8) and (9).

3 Numerical results and discussion

The plasma is assumed to be an Ar discharge plasma and the discharge parameters in the sheath model we used are shown as follows. The rf-bias frequency \( f = 13.56 \) MHz, the typical plasma density \( n_0 = 5 \times 10^{16} \text{ m}^{-3} \), and the electron temperature \( k_B T_e = 3 \) eV.

For the trench domain area, a 200×200 square cellular grid is applied. The dimensionless length of the area \( L \) scaled by the cell length is 200, the depth of the trench \( D = 100 \), and the width of the trench \( W = 30 \), so the aspect ratio (the ratio of the trench depth to the trench width) is confined to 3.3 during this study.

In the following part, different discharge conditions are applied and ion behaviors are studied at pressures of 10 mTorr, 20 mTorr, and 50 mTorr with a fixed amplitude of rf-bias voltage \( V_c = -150 \) V, and also at \( V_c \) of 75 V and 300 V while the pressure \( P \) is fixed to 10 mTorr.

3.1 Influences of the discharge pressure

The initial IEDs and IADs we used as the input parameters for the trench domain are derived from the sheath model. Influences of the discharge pressures on the IEDs and IADs are shown in Fig. 2 and Fig. 3, respectively. We can see that the IEDs have a bimodal shape for the rf sheath, and as the pressure increases, the heights of both peaks decrease due to the ions going through more collisions, especially for the high energy peak. For IADs at different pressures in Fig. 3, the number rate of ions incident normal to the substrate (impact angle \( \approx 0 \)) is not shown in order to exhibit IADs clearly, where the normalized number rate of these ions is 2.588, 1.118 and 0.738 for the pressure of 10 mTorr, 20 mTorr and 50 mTorr, respectively. We can see that, as the pressure increases, ions tend to strike the substrate with larger incident angles. Be-
cause ions undergo a number of collisions with neutrals and are scattered from their original direction during their transport in the sheath, more collisions lead to a more dispersive IADs at larger pressures.

![Fig.2](image1.jpg)  
**Fig.2** Ion energy distributions at different discharge pressures computed from the sheath model

![Fig.3](image2.jpg)  
**Fig.3** Ion angular distributions at different discharge pressures derived from the sheath model. (a) Discharge pressure $P = 10$ mTorr, (b) $P = 20$ mTorr, (c) $P = 50$ mTorr. Number rate of ions incident normal to the substrate (impact angle $\approx 0$) is 2.588, 1.118 and 0.738 in the case of 10 mTorr, 20 mTorr and 50 mTorr, respectively.

In the trench domain, while iterations converge to the steady state, ion fluxes and kinetic energies impacting onto the substrate at different phases of the rf cycle are found and the IEDs and IADs can be calculated using the statistical average of the distributions at all phases of the rf cycle. The normalized distributions are shown in Fig. 4 for the IEDs and Fig. 5 for the IADs, which are computed at the center of the trench bottom; and because the distributions are normalized, the absolute number of ions is different at different pressures.

We can see from Fig. 4 that, when the pressure increases, the IEDs in the trench have similar trends to those in the sheath model: the heights of both peaks decrease, and the influence is more obvious for the high energy peak. But the shape of the distribution functions itself is changed obviously when compared to that in the sheath model, and we can specially compare the IEDs for the sheath model in Fig. 2 with those for the trench model in Fig. 4 at a certain fixed pressure such as 10 mTorr. We can see that, for IEDs in the trench model, more ions tend to have energy larger than that of the low energy peak. We attribute this to the fact that low energy ions are more easily influenced by the local electric field, thus they can strike at the sidewall more easily, and high energy ions tend to reach the bottom. So in the IEDs computed at the trench bottom, ions tend to have an energy in the higher energy region, and this can be a factor that influences the etching profile for a trench.

![Fig.4](image3.jpg)  
**Fig.4** Ion energy distributions by the trench model for different pressures. The statistics are made at the center of the trench bottom.

![Fig.5](image4.jpg)  
**Fig.5** Ion angular distributions for different pressures obtained by the trench model. The statistics are also made at the center of the trench bottom.
Fig. 6 shows the electric potential in the trench domain at three typical phases of the rf cycle, i.e., at \( \varphi = 0, \frac{1}{4}T, \) and \( \frac{1}{2}T \), where \( \varphi \) is the phase of the rf cycle and \( T \) is the period of the rf cycle. We can see the gradient of the potential is larger at the area near the bottom of the trench, and also at the phase near \( \varphi = \frac{1}{2}T \). In addition, we plot the ion trajectories in the trench domain as shown in Fig. 7. Ion trajectories at different phases of the rf cycle are shown for comparison. We can see that ions are under a greater influence near the top entrance of the trench and near the substrate, where the effect is different at different phases of the rf-cycle. At \( \varphi = \frac{1}{2}T \) almost all ions are unable to reach the trench bottom and they are deflected back to the sheath or bulk plasma. We can also see the ion shading effect \([13]\) at the sharp corner of the photore sist layer, and it can be further clearly shown in the ion number distributions at the sidewall of the trench in Fig. 8, where the location number 100 represents the top of the trench sidewall and 200 represents the bottom of the sidewall, and the distribution is scaled by the number of all ions reaching the trench surface. Because of the topography of the trench, the numbers of ions striking the sidewall should decrease with the increase in the depth. However, Fig. 8 shows that at the top of the trench sidewall, like locations numbered between 100 and 105, the ion number is smaller or equal compared to a deeper position of the trench sidewall, such as the location numbered 110; this may be caused by the ion shading effect \([13]\). In this figure we can also see that at higher pressure more ions strike the sidewalls because of their larger incident angles into the trench area. Besides, the ion number at the bottom of the sidewall is slightly increased and it may be relevant to the notching effect caused by the charging effect \([18]\).

![Fig. 6](image_url) Electric potential at different phases of the rf cycle with the fixed pressure \( P = 10 \) mTorr

3.2 Influences of amplitude of the rf-bias

The ion trajectories or potential distributions for different amplitudes of rf-bias are similar to the figures above. So we only present the IEDs and IADs through the sheath model and trench model, respectively, to show the influences of the addition of the photoresist trench at different rf-biases.

![Fig. 7](image_url) Ion trajectories at different phases of the rf cycle at 10 mTorr

![Fig. 8](image_url) Ion number distributions at different locations of the trench sidewall at different pressures. Location number 100 represents the top of the trench sidewall and 200 represents the bottom of the sidewall

Fig. 9 shows the IEDs at different rf-biases derived from the sheath model, where we can see the increase in the rf-bias makes both peaks move to the high energy region, and the width between the two peaks is enlarged because the high energy peak moves more. In Fig. 10, IADs at different rf-biases are shown. As in
Fig. 3, the number rate of ions normal to the substrate (impact angle $\approx 0$) is not shown, where the normalized number rate is 2.604, 2.588 and 2.590 in the case of 75 V, 150 V and 300 V for the rf-bias, respectively. Although not obvious, we can still find that at higher rf-bias, the number of ions incident at a small angle (less than 5 degrees) normal to the substrate increases while the number of ions incident at a larger angle decreases. That is because the ion directional velocity after passing through the sheath is increased as ions are accelerated in the increased voltage drop of the sheath; besides, from Eqs. (6) and (7) we can find that at a larger ion kinetic energy, the cross sections decrease for both elastic collisions and charge exchange collisions, and with fewer collision processes, ions tend to have a better mono-directional property.

Fig. 9 Initial IEDs at different amplitudes of rf-bias computed from the sheath model

Fig. 10 Initial IADs computed from the sheath model at different rf-biases. (a) $V_c=75$ V, (b) $V_c=150$ V, (c) $V_c=300$ V. Number rate of ions incident normal to the substrate (impact angle $\approx 0$) is 2.604, 2.588 and 2.590 in the case of 75 V, 150 V and 300 V, respectively

Fig. 11 IEDs from the trench model at different rf-biases

Fig. 12 IADs from the trench model at different rf-biases

Fig. 13 Ion number distributions at different locations of the trench sidewall at different rf-biases
4 Conclusion

With the charging effect of the photoresist considered, a one-dimensional sheath model and a two-dimensional trench model are coupled to study ion transport behaviors near and in the trench in an rf-CCP discharge plasma.

From the sheath model, we can see that, as the pressure increases, the heights of both peaks in the IEDs decrease, and ions tend to have smaller impact energies and larger impact angles normal to the substrate. Also, as the amplitude of the rf-bias increases, both peaks in the IEDs move to the high energy region, and the movement of the peak with high energy is greater. Ions tend to have smaller impact angles normal to the substrate.

Numerical results also show that, because of the existence of the trench, in IEDs there have more ions that have larger impact energies, and this is because the low energy ions are more easily influenced by the local electric field and can more easily reach the trench sidewall instead of the bottom.

With the increase in the pressure, the heights of both peaks decrease, but the height of the high energy peak decreases more. Ions tend to have smaller impact energies. As for the distributions of the ion angles, the fraction of ions with a large impact angle increases significantly.

With the increase in the amplitude of the rf-bias, the heights of both peaks decrease and the high energy peak is lowered more seriously in IEDs. The tendencies of IADs are similar to those in the sheath model.

In addition, at the entrance of the trench, the ion orbits are distorted and the ion shading effect is observed.

In our future work, we will further consider the reflection of the ions on the sidewalls, the application of a dual-frequency source, etc. In addition, by considering the chemical etchant and etch yield, we can further simulate the evolution of the etching profile.

References


(Manuscript received 3 May 2011)
(Manuscript accepted 21 February 2012)
E-mail address of corresponding author DAI Zhongling: daizhl@dlut.edu.cn