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Phasespace modelling of a radiofrequency plasma interacting with surfaces

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Abstract: A parallel plate capacitively coupled plasma (CCP) exhibits the fundamental property for dry etching. Local excess charging is one of the causes of damage to ULSI circuit fabrication, i.e., anomalous etching and electrical breakdown of the gate oxide. A pulsed operation of the CCP will provide charging free processes for etching. The interface between a pulsed plasma and a microstructure on a wafer is investigated by the relaxation Continuum/Boltzmann equation model. The capability of the pulsed plasma for producing a drift electron wave and negative ions to the wafer surface is demonstrated and discussed.

Introduction

Traditional parallel plate capacitively coupled plasma (CCP) at 13.56 MHz exhibits the fundamental characteristics required for dry etching. Extended two-frequency CCP assumes the lead in the etching efficiency of SiO_2 in microelectronic device fabrication. Recently, a pulsed operation of the CCP is proposed to realize the charging free plasma processing for etching. A large scale uniform plasma has two major characteristics equalities in a steady state condition. That is,

/1/the positive ion density is equal to that of the negative charges in the bulk plasma, and

/2/at any boundary the positive ion current incident on the surface is identical to the current of the negative charges.

Dry processes on a nanometer scale are carried out under the conditions of these two physical equalities on a large scale. The nonequilibrium plasma for etching is also characterized by the presence of negative ions. Due to the large difference in mass between the electron and the ion, the surface of an insulator or electrically isolated conductor is always negatively charged in a steady state. In a high aspect ratio hole or trench, however, electron shading, due to the isotropic velocity distribution, and a topographical surface structure causes a positive charging on the bottom of the etched surface. A local excess charging with positive polarity is one of the candidates for two different types of significant damage to ULSI circuit fabrication, i.e., anomalous etching and the electrical breakdown of the gate oxide$^{1)}$(see Fig. 1). The characteristics of the ion velocity distribution incident on a high aspect ratio structure play a key role in the anomalous etching, i.e., local side etching (notching)$^{2)}$ and microloading (RIE-lag), under a local heteropolarity on an etched surface.

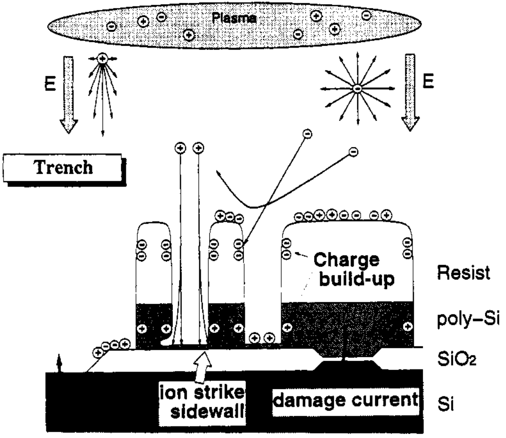

Figure 1: Anomalous etching and gate oxide damage by charge buildup in plasma processes.

A number of experimental and numerical studies aimed at improving the etched profile have been performed in a high aspect ratio structure in the last several years. Some probable scenarios have been put forward to reduce the anomalous etching caused by the topography-dependent charging in dry processes. The first scenario is the positive bias pulse operation with a very short risetime on the order of 10 ns on the wafer under a continuous plasma source3). This technique was originally intended to produce beam-like electrons incident perpendicular to the wafer surface. The second scenario is the use of pulsed plasma in the intermediate range of $10\mu s$-$100\mu s$ with a low frequency bias voltage on the wafer surface4). The intent is to neutralize the surface with a large number of negative ions produced by electrons with lower energy in the afterglow phase of the pulsed plasma. Lowering the electron temperature in plasmas is the third way to reduce the sheath potential and to increase the lower energy positive ions on the wafer. The first two experimental proposals suggest that *it is important to investigate the transient phenomena in the close vicinity of the wafer immersed in the plasma.* Very recently, a measurement of intrinsic electron shading damage was carried out by using SiO_2 mask pattern instead of the usual photoresist, which may produce a profile transition or redeposition inside of the microstructure5). A polysilicon overetching process in a high aspect ratio structure was simulated under the assumption of internal pulsed plasma parameters, i.e., sheath potential and the related energy distribution of positive ions and electron temperature in the bulk plasma without considering a transient time between the on/off mode. The series of investigations yielded the conclusion that the bottom surface potential will be controlled by the sheath potential in off-mode in the steady state6). The electron and ion dynamics from a high density continuous plasma has been simulated in the microstructure under low frequency bias voltage at 400 kHz, and with the profile evolution being simulated predicting the notching combined with ion dynamics on the inner etched surface7).

Under these circumstances, a comprehensive understanding of charging damage requires a detailed modeling of electrons, and positive and negative ions in a whole system including a bulk plasma, positive ion sheath and topographic microstructure. In particular, the transient behavior after the plasma is switched off must be clarified. In this paper, we present a system of phase space modeling that is capable of predicting the transient phenomena of the plasma etching system. The practical validity of a pulsed plasma source with a bias pulse operation will be discussed with respect to a capacitively coupled plasma in SF_6.

Theoretical approach

The relaxation continuum (RCT)/Boltzmann equation model has been developed for use in plasma simulation in phase space8). In the present paper, the RCT/Boltzmann equation model is applied to the interface between a plasma and a microstructure on the wafer in order to study the phase space behavior of electrons. The numerical calculation under the governing equations of the RCT model9) is carried out first to guess the rf pulsed-plasma characteristics in position space. By using the plasma characteristics as an initial guess, the RCT/Boltzmann equation is analyzed in order to obtain the final phase space characteristics. We consider the Boltzmann equation for electrons in one-dimensional position space with a field direction of z and in two-dimensional velocity space with spherical coordinates $\boldsymbol{v} = (v, \theta, \phi)$ in an electrode system with flat parallel plates (See Fig.1) as,

$$\frac{\partial}{\partial t} G(z, \boldsymbol{v}, t) + \boldsymbol{v} \cdot \frac{\partial}{\partial z} G(z, \boldsymbol{v}, t) - \frac{e\boldsymbol{E}(z,t)}{m} \cdot \frac{\partial}{\partial \boldsymbol{v}} G(z, \boldsymbol{v}, t) = \boldsymbol{J}(G, F), \tag{1}$$

where, $G(z, \boldsymbol{v}, t)$ is the phase-space distribution function of electrons. The integration with respect to $\boldsymbol{v}$ gives the number density, $n_e(z,t)$. e and m are, respectively, the charge and the mass of the electron, $\boldsymbol{E}(z,t)$ the instantaneous local field, and $\boldsymbol{J}$ denotes the term for collision between the electron and the molecule. We write the phase-space distribution function of the electrons at position z_i, velocity magnitude v_j and the polar angle θ_k at time t by

$$G(z_i, v_j, \theta_k; t), \tag{2}$$

because the velocity space is axisymmetry with respect to v_z. The boundary conditions of $G(z, v, \theta; t)$ are given in velocity and position spaces.

$$G(z, v, \theta)|_{v > v_{max};t} = 0, \tag{3}$$

where v_{max} satisfies the relation

$$\frac{G(v_{max})}{\mathrm{Max}[G(v)]} \leq 10^{-6}. \tag{4}$$

None of the other boundary conditions in velocity space are required even in the origin, $v = 0$, in the present *shift*-and-*scattering* in V-space and *shift* in R-space algorithm(SSSA). In position space, we assume a perfect absorbing boundary of electrons.

$$G(z, v, \theta; t)|_{z=0} = G(z, v, \theta; t)|_{z=d} = 0. \tag{5}$$

This will be satisfied by a high frequency discharge, sustained by an electron impact volume ionization.

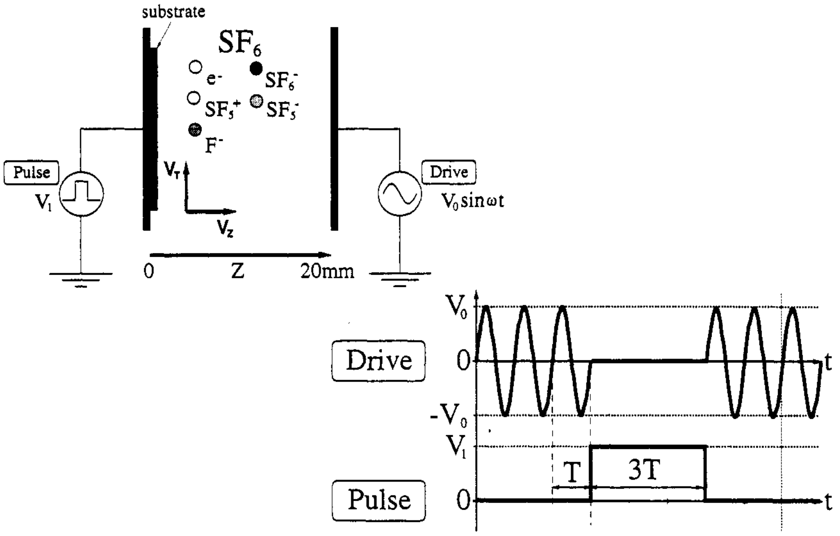

Figure 2: Pulsed CCP reactor and time sequence of the power source and bias voltage.

Results and discussion

A capacitively coupled plasma is maintained between parallel plates with 2 cm separation by a pulsive operation at an rf power source with frequency of 13.56 MHz and amplitude of 250 V at 0.1 Torr in SF_6. The substrate opposite is driven by square waves with an amplitude of 250 V during the off-period of the rf power source (see Fig. 2). In this study, a duty ratio, defined by the ratio of the on-time to the total period, of 17/20, has been employed. A periodic steady state pulsed-discharge, then, is maintained between both electrodes with a plasma density of $10^{10}\mathrm{cm}^{-3}$.

Figure 3 shows the typical spatiotemporal profile of the potential formed by the pulsed operation of a plasma source with the bias voltage application synchronized with the rest period (see Fig. 2). It will be essential to controlling the space potential close to the wafer as a function of duty ratio, bias pulse amplitude. As shown in Fig. 3(a), there exists great difference between on- and off-mode of the power source. That is, the potential profile to accelerate electrons toward the wafer is gradually formed during the off-peiod of the plasma source, while the field to accelerate ions or decelerate electrons to the wafer is kept during the on-period of the plasma source. During the bias pulse operation in the afterglow phase, the electron in the bulk plasma migrates to the wafer as shown in Fig. 3(b). The origin of the electron migration as a *drift wave* lies in the sudden change of the applied power source, i.e., in the break. This causes the plasma instability over the whole space between both electrodes, and the instability propagates through the bulk plasma to the bias electrodes as the electron drift wave. When a continuous voltage wave at low frequency is applied to the wafer, instead of the unipolar bias pulse, the instability propagates alternately both to the powered electrode and to the bias electrode with low frequency.

During the migration of electrons, the negative ion F^- is produced by the dissociative attachment of the front electrons with higher energy component with SF_6, as welll as the neutralization of the positive ion sheath in front of the wafer. As a result, the appreciable degree of negative ions F^- and the apparent drift to the wafer are observed as shown in Fig. 3(c). Even in the phase after the bias pulse is switched off, F^- continues to propagates to the wafer. This will give the mechanism which controls the showers of electrons and negative ions on the wafer surface with the bias voltage, when the plasma is in pulsed operation.

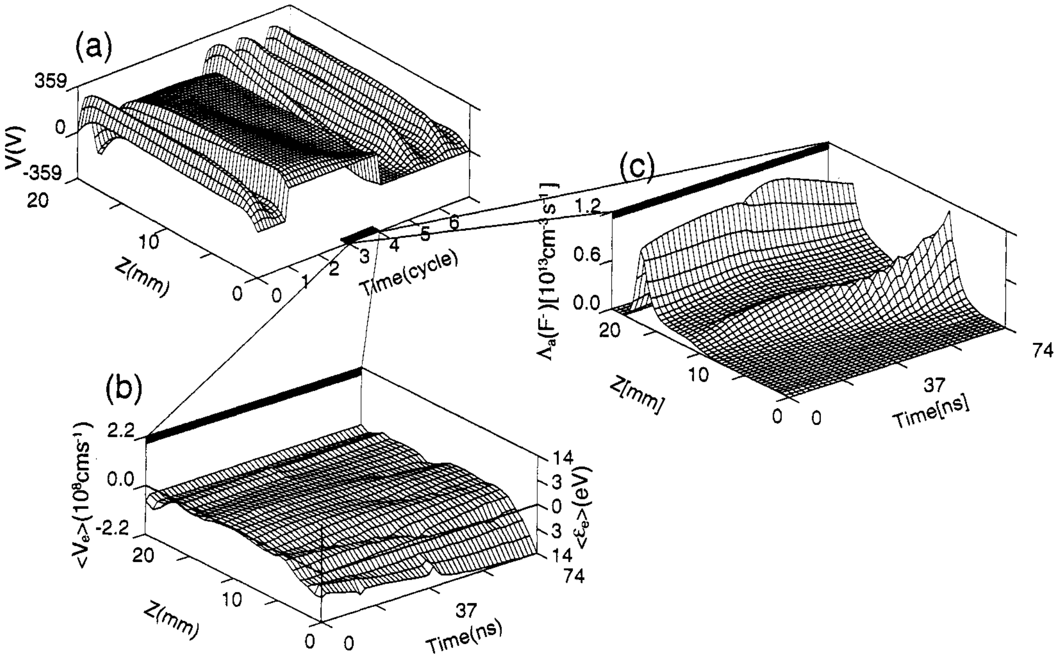

Figure 3: Spatiotemporal characteristics of the potential, electron drift velocity, and net production rate of negative ion F^-. External conditions are in the text.

The characteristics of the *electron drift wave* in the pulsed plasma are further investigated by the phase space analysis using the Boltzmann equation. The temporal profile of the velocity distribution of electrons in a bulk plasma in an rf periodic steady state in the on-time was previously studied[10)]. The appearance of the anisotropy and the higher order Fourier components in $G(z, \boldsymbol{v}, t)$ during one period have been discussed in detail. The transient characteristics of $G(z, \boldsymbol{v}, t)$, at $z=$ 1.2 mm from the wafer surface are shown in Fig. 4 at the four different phases, 0.875, 1.875, 2.875, and 3.875 cycles in Fig. 3(a). This corresponds to the macroscopic plasma response in SF_6 under the present pulsed-plasma condition. The almost isotropic velocity distribution in the on-time of the rf power gradually changes its shape to a function with a strong directional velocity component in relation to the substrate in the off-time. The beam-like electron is formed close to the wafer at Fig. 4(d). The velocity distribution strengthens the beam-like component to the wafer, with the electron flux incident on the substrate decreasing. This is a result of the collapse of the strong positive ion sheath field, causing in part by the external bias voltage during the phase from 1 to 4 cycles. In compensation for the neutralization of the space close to the substrate by the large number of electrons, the electron is almost exhausted in the period of its acceleration towards the substrate. The lower limit of the electron density to keep a periodic steady state plasma condition is the order of 10^7 cm^{-3} in the bulk plasma just befor the switching on of the rf power.

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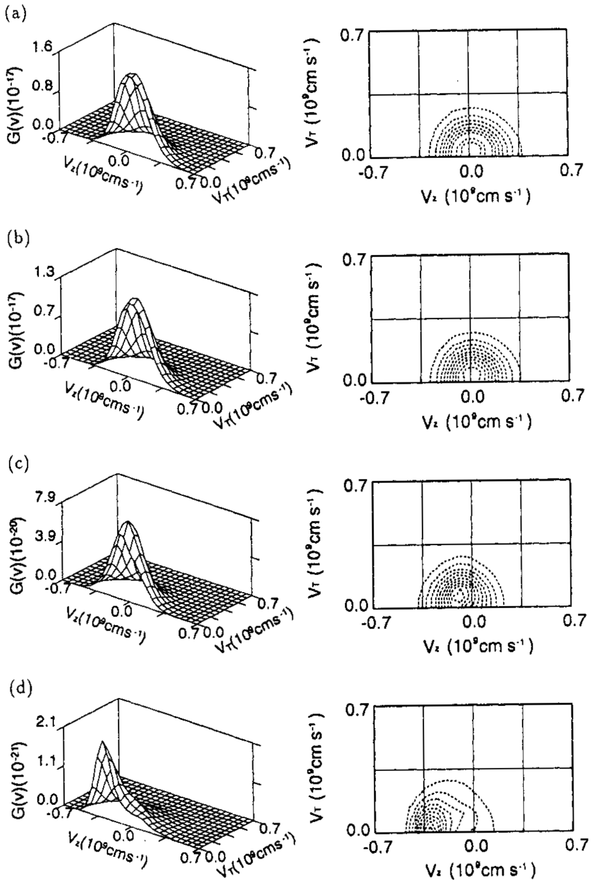

Figure 4: Two dimensional velocity distribution of electrons at 1.2 mm from the wafer at four phases, 0.875(a), 1.875(b), 2.875(c), and 3.875(d) cycles in Fig.3(a)[8]. External conditions are in the text.

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