Effect of collisions on ion dynamics in electron-cyclotron-resonance plasmas

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A one-dimensional kinetic code is used to study the effect of ion-neutral (charge exchange and elastic scattering) and ion-ion collisions on plasma flow in the downstream region of an electron-cyclotron-resonance plasma etching system. Ions are assumed to leave the source region at the Bohm velocity. Argon, nitrogen, and CF_4 plasmas are simulated, assuming that the dominant ion species are Ar^+ , N_2^+ , and CF_3^+ , respectively. Results show that charge exchange and elastic scattering collisions play a significant role in reducing the electrostatic potential variation in the downstream region. For neutral gas pressures above ~ 1 mTorr, the potential drop in the downstream region is small, which means that most of the energy with which ions hit the substrate surface is gained while crossing the substrate sheath region. Although the effect of ion-ion collisions on the plasma potential profile and on the ion distribution function is weak, ion-ion collisions are responsible for transferring energy from the parallel to the perpendicular direction and hence increasing the perpendicular ion temperature.

I. INTRODUCTION

In a typical electron-cyclotron-resonance (ECR) microwave plasma etching system, microwave power is introduced into the source region through a quartz window, as illustrated in Fig. 1. The microwave power is coupled to the plasma at the ECR frequency, generating energetic electrons which ionize, dissociate, and excite the neutral gas present. Ions produced in the source region are accelerated by the static, self-generated potential to the downstream region. It is believed that better process capabilities and control can be achieved in an ECR plasma etching system through accurate control of the ion energy impinging upon a substrate. Experimentally it has been shown that in an ECR microwave etching plasma, the ion energy and flux density can be controlled independently of the gas pressure by controlling the magnetic-field gradient.¹ Although ECR systems are being used in etching, deposition, and other plasma-aided manufacturing processes, the present understanding of the physics of such systems is far from complete.

Measurements of the ion energies in ECR plasmas have been made and reported by many investigators. Matsuoka and Ono measured the ion energy distribution at the substrate in an argon plasma using a gridded ion energy analyzer.² In contrast to Matsuoka and Ono, Holber and Forster³ measured the impact ion energy on both floating and rf-biased substrate plates using a nongridded ion energy analyzer. Hopwood, Reinhard, and Asmussen⁴ measured both the electron and ion energy distribution functions in the downstream region of a multipolar ECR plasma using an ion impingement energy analyzer. All groups reported similar results. The peak ion energy, the width of the ion energy distribution, and the electrostatic

potential drop all decrease with increasing neutral gas pressure.

Sadeghi *et al.*⁵ reported detailed measurements of the metastable ion velocity distributions in both the source and downstream regions of an ECR plasma etching system. They used Doppler-shifted laser-induced fluorescence (LIF) spectroscopy to measure the metastable argon-ion velocity distribution parallel and perpendicular to the magnetic field. A bimodal metastable ion velocity distribution was observed in the downstream region. Den Hartog, Persing, and Woods⁶ reported LIF measurement of the transverse ion temperature $T_{\perp}$ of ground state N_2^+ in an ECR nitrogen plasma. The value of $T_{\perp}$ was determined from the measured width of the Doppler-broadened transition and was found to decrease with increasing neutral pressure. The analysis of further LIF measurements of both $T_{\perp}$ and $T_{\parallel}$ by Den Hartog *et al.*⁷ have suggested that ion-ion collisions may also play an important role in the ion dynamics of ECR etching plasmas.

On the other hand, attempts to model ECR plasmas have been very limited. Porteous and Graves⁸ used a hybrid electron fluid-particle ion model to simulate the plasma flow in a cylindrical axisymmetric discharge in two spatial dimensions. On the contrary, Weng and Kushner⁹ used a model that is based on a Monte Carlo description for the electrons and a fluid treatment for the ions. They concentrated on examining the transport of hot electrons from the ECR zone to regions near the substrate.

In a previous work,¹⁰ we presented a numerical simulation technique to model the plasma flow in the downstream region of an ECR reactor. The simulation was based on a kinetic description for the ions and a fluid treatment for the electrons. The effect of the magnetic-field profile on the ion dynamics in the downstream region was the major issue addressed in that work. The effect of neutral gas pressure was examined only over a very narrow range of pressure. In this work, we attempt to give a better un-

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FIG. 1. The layout of the ECR plasma etching experiment modeled in this work. Also shown is the computational grid used in the simulation.

understanding of the energetics of the ionic species in ECR discharges. The main focus of the present work is on studying the effects of ion-neutral collisions (charge exchange, elastic scattering) and ion-ion Coulomb collisions on the ion dynamics, electrostatic potential formation, and ion energy distribution function in the downstream region.

II. SIMULATION MODEL AND ASSUMPTIONS

Steady-state plasma flow along the divergent magnetic field of the downstream region of an ECR plasma etching reactor is determined by the kinetic equation for ions,

$$\mathbf{v} \cdot \nabla f_i + \frac{\mathbf{F}}{m_i} \left(\frac{\partial f_i}{\partial \mathbf{v}} \right) = S + \left(\frac{\partial f_i}{\partial t} \right) c, \quad (1)$$

where $\mathbf{F}$ is the force on an ion with mass m_i , velocity $\mathbf{v}$, and a distribution function f_i , S is the source term for these ions, and $(\partial f_i / \partial t) c$ is the rate of change of the ion distribution function due to collisions. Quasineutrality along a field line outside the sheath region requires that

$$en_e(x) = qn_i(x) = q \int f_i d\mathbf{v}, \quad (2)$$

where n_e and $-e$ are the density and charge of the electrons, and n_i and q are the density and charge of the ions. We assume that the electrons are represented by a Boltzmann distribution

$$n_e(x) = n_{e0} \exp \left(\frac{e\Phi(x)}{kT_e} \right), \quad (3)$$

where $\Phi(x)$ is the electrostatic potential, n_{e0} is the electron density at $x=0$, where Φ is defined to be zero, and k is the Boltzmann constant.

Instead of calculating the ion density from the ion distribution function f_i , obtained by solving the kinetic equation, our approach is to determine the ion density indirectly by computing ion trajectories in the self-produced electrostatic potential and the externally applied magnetic field. Plasma streaming out of the source region along magnetic-field lines is modeled by a single particle flux source at $x=0$, as shown in Fig. 1, which also illustrates the computational mesh used in this work. Assuming that ions leave the source region with an average velocity given by the Bohm velocity $C_s = \sqrt{(T_e + T_i)/m_i}$, the particle source at $x=0$ emits particles with random perpendicular velocity $v_\perp$ sampled from a Maxwellian distribution and random parallel velocities sampled from a shifted 1D Maxwellian distribution given by

$$f(v_\parallel) = \sqrt{(m_i/2\pi kT_i)} \exp[-(m_i/2kT_i)(v_\parallel - C_s)^2]. \quad (4)$$

The time these ions spend in a given volume element determines the ion density. This can be thought of as an indirect solution of the kinetic equation. A trajectory is terminated, and a particle is lost whenever it hits the substrate at $x=L$, which is assumed to be electrostatically floating and perfectly absorbing. The ion density is used in the quasineutrality relation, Eq. (2), and the electrostatic potential Φ is then determined from the Boltzmann relation, Eq. (3). We iterate until a convergent potential profile is reached. The details of the numerical algorithm used here were reported earlier.¹¹

In the downstream region of an ECR source, the electron temperature T_e is only a few eV. Any ionizations are caused by the tail of the electron energy distribution. Assuming that the number of these energetic electrons is small, and that the number of cold ions produced from their ionizing collisions with the neutral gas is negligible compared to the input ion flux at $x=0$, only charge-exchange and elastic scattering collisions between ions and neutrals need to be considered. In a real experiment, however, $\sim 10\%$ or more of the ion density in the downstream region may be due to hot-electron ionizations at low pressure. This ratio varies with neutral gas pressure.¹²

III. COLLISION MODEL

Three types of collisions are being considered here: charge exchange, ion-neutral elastic scattering, and ion-ion Coulomb scattering. The collision dynamics is studied in a three-dimensional velocity space using a Monte Carlo treatment.¹³ Ion trajectories are computed using the guiding center approximation with finite gyroradius effects included in the calculation of the path length used in computing the collision probability. The path length estimator method¹⁴ is used to determine whether a collision event will occur in any given cell. The collision model is struc-

tured in such a way that all collisions are treated in the same manner. It should be noted, however, that Coulomb collisions are not really true collisions (in the sense of instantaneous collisions). Because of the long range of the Coulomb force, the stochastic interaction between charged particles goes on continuously and causes a continuous randomization of particle velocity.

A. Ion-neutral collisions

Our treatment of elastic scattering collisions between ions and neutrals follows the standard Monte Carlo approach for this type of collision.¹³ Elastic scattering is assumed isotropic in the center-of-mass (COM) frame. In a charge-exchange collision between an ion and a neutral, we assume that only the charge is transferred from the ion to the neutral during the course of the collision. The velocity components of a neutral particle at a collision site are chosen randomly. The parallel velocity component of the interacting ion is determined from its motion along a field line, while the perpendicular component is computed from the invariance of the magnetic moment $\mu = m_i v_{\perp}^2 / 2B$, where $v_{\perp}$ is the ion perpendicular velocity. The postcollision velocity components of the ion to be followed after a charge-exchange collision are those of the interacting neutral particle before collision. Heating of the neutral gas due to such collisions is ignored at the present time. Neutral heating effects, however, are not expected to significantly influence the results obtained.

The cross sections for elastic and charge-exchange collisions between ions and neutrals at low ion energies are calculated using a classical model. The potential field between an ion and a molecule is assumed to be the inverse-fourth-power polarization potential given by¹⁵

$$V(r) = -\alpha q^2 / 2r^4, \quad (5)$$

where α is the electric polarizability of the molecule and q is the ionic charge. Polarizabilities for atoms and molecules used in this work are obtained from Ref. 16. The collision cross section at low energy calculated for this potential is

$$\sigma = (2\pi / v_r) \sqrt{\alpha q^2 / M_r}, \quad (6)$$

where M_r is the reduced mass of the interacting ion and molecule and v_r is their relative velocity. At higher energies, however, the model predicts that the cross section falls to zero, whereas it should actually drop to πr_c^2 , where r_c is the radius of the molecule (atom). An alternative expression which is used at higher energies and holds for attractive or repulsive potentials is derived in Ref. 15 as

$$\sigma = \pi r_c^2 \left(1.0 - \frac{2V(r_c)}{M_r v_r^2} \right). \quad (7)$$

This equation applies to energies above a certain threshold value, which is equal to the potential energy evaluated at the radius r_c . Based on the nature of collisions in the polarization potential, namely orbiting collisions, we assume that once a collision occurs there is an equal chance for either a charge exchange or an elastic scattering reaction. Therefore, the cross section for both reactions is the collision cross section calculated from Eq. (6) or Eq. (7).

It is important to note that in the case of nitrogen and argon where resonant charge-exchange collisions dominate, the experimental cross sections exceed those predicted by the above equations. Therefore, the mean free paths at a given pressure are shorter and collisional effects are probably even greater than predicted here. For a $\text{CF}_3^+ / \text{CF}_4$ system, the cross sections are less well known experimentally, but the simple polarization model should be more accurate.

B. Ion-ion collisions

The treatment of ion-ion collisions is based on a Monte Carlo binary collision model. Assume a collision between two interacting ions, which we call a test ion and a field ion. The test ion (1) is the one being followed, therefore its velocity components are known. The second ion (2) is the field ion. The question now is how to choose the velocity components of this field ion. Takizuka and Abe¹⁷ developed an algorithm for simulating Coulomb collisions that partially answers this question. A modification of that algorithm is used in our present work.

The velocity components of the field ion 2 are chosen from a stored velocity matrix. Such a matrix exists for both the parallel and the perpendicular components. Initially, the velocity matrix contains velocities sampled from the probability distribution given by Eq. (4). If an ion-ion collision is to occur, both $v_{\parallel}$ and $v_{\perp}$ are chosen randomly from the corresponding velocity matrix. The relative velocity of the two interacting ions is then computed and the collision dynamics is studied in the COM frame. Although the magnitude of the relative velocity does not change in the COM frame as a result of the collision, its direction is altered by an angle Θ . The velocity components after collision are then transformed back into the laboratory frame. Due to the random nature of Coulomb collisions, $\tan \Theta/2$ can be chosen randomly from a Gaussian distribution with zero mean and variance given by¹⁷

$$\text{variance} = \left(\frac{q_1^2 q_2^2 n_i \ln \Lambda}{8\pi \epsilon_0^2 m_{12}^2 u^3} \right) \Delta t, \quad (8)$$

where $m_{12} = m_1 m_2 / (m_1 + m_2)$, and the subscripts 1 and 2 label the test and field ions, respectively. The symbol u denotes the magnitude of the relative velocity. The time interval Δt is taken as the time to collision within a given cell. If the variance given by Eq. (8) exceeds unity, the scattering angle Θ is chosen randomly with a uniform distribution between 0 and π .

After the collision, the trajectory of ion 1 is followed starting from the collision site with initial velocities given by the postcollision velocity components. To take into account the effect of the collision on the field ion 2, its postcollision velocity components are also computed and the velocity matrix is updated accordingly.

IV. EFFECT OF ION-NEUTRAL COLLISIONS

The following results are obtained for argon, nitrogen, and CF_4 plasmas assuming that the dominant ion species are Ar^+ , N_2^+ , and CF_3^+ , respectively. Our assumption that

FIG. 2. The variation of the plasma potential profile with neutral pressure for CF_4 plasma.

CF_3^+ is the predominant ion in a CF_4 plasma is based on the experimental observations reported in Refs. 18 and 19, which were performed in a rf system. The high power densities usually associated with microwave ECR heating of a plasma, however, could produce other significant ionic species. We consider a simulation length $L=0.7$ m and the divergent magnetic-field profile shown in Fig. 1. We assume that neutrals are cold and $T_e/T_i=8$. For convenience, we introduce the normalized distance $X=x/L$. The results presented in this section are derived considering only charge-exchange and elastic scattering collisions.

A. Plasma potential profile

The potential drop across the downstream region decreases as the neutral gas pressure increases. Figure 2 shows the variation of the spatial profile of the plasma potential in the downstream region plasma with neutral gas pressure for CF_4 . Similar potential profiles are obtained for argon and nitrogen plasmas. When an ion-neutral collision takes place (charge exchange or elastic scattering), a hot ion is replaced by a colder one, since the neutral gas is assumed to be at room temperature. In an elastic scattering collision, an ion loses, on the average, half of its initial energy before collision. Energy transfer in charge-exchange collisions is even more severe because an ion loses all its energy and is replaced by a colder one. As the ion energy decreases, its transit time increases, giving rise to an increased ion density in the downstream region compared to that obtained with no collisions. The variation in the density profile determines the electrostatic potential. For quasineutrality to be satisfied, the electrostatic potential must increase accordingly. For neutral gas pressures above ~ 1 mTorr, the change in the electrostatic potential practically vanishes. The impact of these changes in the plasma potential profile on the ion energy spectrum are discussed later.

It should be noted that the boundary at $X=1$ is placed on the plasma side of the substrate sheath edge. The simulation does not enter the sheath itself, which is assumed to be ion attracting. Since the substrate is electrostatically floating, the requirement of equal ion and electron fluxes to the substrate surface determines the floating potential Φ_f . That is,

FIG. 3. The variation of the electrostatic potential drop across the substrate sheath with neutral gas pressure.

$$\Phi_f = (kT_e/e) \ln[(\Gamma_i/n_{e0}) \sqrt{2\pi m_e/kT_e}], \quad (9)$$

where m_e is the electron mass and Γ_i is the ion flux at the sheath edge. The potential drop across the sheath is given by $\Phi_f - \Phi_s$, where Φ_s is the potential at $X=1$. As shown in Fig. 3, the sheath drop normalized to the electron temperature increases with neutral pressure. This is a direct result of the reduction in the plasma potential drop in the downstream region as the neutral gas pressure increases. Note that the floating potential, as computed from Eq. (9), does not change with pressure, since the ion flux and the electron temperature are taken to be the same at all pressures considered in the simulation. In a real experiment, however, this is not true. The electron temperature and the ion flux streaming out of the source region are both functions of neutral gas pressure.

B. Ion parallel energy spectrum

We start by examining the spatial behavior of the ion energy spectrum as ions move along a magnetic-field line from the source throat to a wafer surface in the downstream region. The ion parallel energy spectrum at three different locations ($X=0, 0.4$, and 1) on the axis of the

FIG. 4. The spatial variation of the parallel ion energy distribution in argon plasma at 0.8 mTorr.

FIG. 5. The variation of the ion parallel energy spectrum at the substrate sheath edge with neutral pressure for a nitrogen plasma.

device is shown in Fig. 4 for an argon plasma at 0.8 mTorr. Similar changes in the energy spectrum are also observed in nitrogen and in CF_4 plasmas. Ions are born with the ion energy spectrum at $X=0$ shown in Fig. 4. As they flow along the magnetic-field line, ions collide with the neutral gas atoms (molecules) in charge-exchange and/or elastic scattering collisions. As explained in Sec. IV A, charge-exchange and elastic scattering collisions produce low-energy ions. This results in the buildup of two distinct peaks in the energy spectrum at low pressure. Focusing on the spectrum at $X=0.4$, the sharp low-energy peak is produced by ions that emerged from collisions near $X=0.4$, so that they did not have the chance to gain any energy from the self-produced electric field. The second peak is centered about an ion energy that corresponds to the energy gained by the ions from the electrostatic potential in flowing, without collisions, along the magnetic-field line from $X=0$ to $X=0.4$. The part of the spectrum in between is produced by those ions that experienced one or more collisions and were accelerated to some extent by the electric field. As ions travel towards the sheath edge at $X=1$, the probability of undergoing a collision increases and, hence, the number of ions that reach the sheath without making a collision decreases. This results in changing the relative height of the two peaks.

The behavior of the ion energy spectrum with neutral gas pressure is illustrated in Fig. 5, which shows the ion energy spectra in a nitrogen plasma at different neutral pressures. At low pressure, the spectrum is characterized by the existence of a single peak: the high-energy one. As pressure increases, collisionality increases, and the low-energy peak starts to build up according to the above argument. Therefore, as a result of ion-neutral collisions the ion energy with which an ion hits the substrate is practically the energy gained in crossing the substrate sheath. The ion energy spectrum, as shown in Fig. 6, incident on the substrate is that at the sheath edge increased by the amount of energy gained in crossing the sheath.

The variation of the ion average parallel energy at the

FIG. 6. The variation of the ion parallel energy distribution incident on the substrate surface with neutral pressure for CF_4 plasma. The energy gained in crossing the sheath is included.

sheath edge $\langle E_{\parallel} \rangle$ with neutral gas pressure is given in Fig. 7 for the three gases under consideration. It is clear that $\langle E_{\parallel} \rangle$ decreases as the pressure increases due to charge-exchange and elastic scattering collisions with the neutral gas.

C. Ion perpendicular velocity spectrum

In this section, we choose to illustrate the effect of ion-neutral collisions on the perpendicular motion by examining the velocity rather than the energy spectra since this better reveals the differences in the spectrum. The ion perpendicular velocity $v_{\perp}$ is computed from the invariance of the magnetic moment of the ion. At $X=0$, each particle is assigned $v_{\perp}$ from which the magnetic moment is computed. Only collisions can change this initial value of the magnetic moment. Figure 8 shows the spatial variation of the ion perpendicular velocity spectrum in nitrogen at 0.5 mTorr. The spectrum at $X=0$ is the initial distribution from which ions are assigned their $v_{\perp}$. As ions flow along the divergent magnetic-field line, their perpendicular velocity is transferred into the parallel direction, as dictated by the invariance of the magnetic moment. On the other hand,

FIG. 7. The variation of the ion average parallel energy at the sheath edge with neutral gas pressure for argon, nitrogen, and CF_4 .

FIG. 8. The spatial variation of the ion perpendicular velocity spectrum in a nitrogen plasma at 0.5 mTorr.

collisions will reduce $v_{\perp}$ as well. However, as illustrated in Fig. 9, the effect of pressure on the perpendicular velocity spectrum is not as significant as on the parallel velocity distribution. The expansion of the magnetic-flux tube is the main reason behind the changes in the perpendicular velocity spectrum.

The angle by which ions impinge on the substrate surface is given by $\tan^{-1} [v_{\perp}(s)/v_{\parallel}(s)]$, where $v_{\perp}(s)$ and $v_{\parallel}(s)$ are the ion perpendicular and parallel velocities at the substrate surface, respectively. The parallel velocity of an ion hitting the substrate is given by its value at the sheath edge plus the velocity acquired in crossing the sheath. The perpendicular velocity, on the other hand, does not change in crossing the sheath, since the sheath is thin and may be assumed collisionless. Therefore, $v_{\perp}(s)$ is assumed to be the same as at the sheath edge. Since an accurate calculation of the ion angular distribution at the substrate surface requires an accurate calculation of the floating potential, computing the correct angular distribution is contingent upon our knowledge of the variation in the electron temperature, and the ion flux at the source throat with neutral gas pressure.

FIG. 9. The variation of the ion perpendicular velocity spectrum at the substrate sheath edge with neutral pressure. The working gas is CF_4 .

FIG. 10. Effect of ion-ion collisions on the plasma potential profile. The working gas is argon.

V. EFFECT OF ION-ION COLLISIONS

The calculations for which results are presented in this section were aimed towards examining the effect of ion-ion collisions on ion dynamics in the downstream region. The degree of collisionality of the system is expressed in terms of the mean free path for ion-ion collisions normalized to the length of the simulation region. All the results presented in this section are for an argon plasma with ion-ion collisions as the only possible type of collision. This enables us to isolate the effects of Coulomb collisions and provide an understanding of the relative importance of such collisions. We assumed $T_e = 0.6$ eV.

First, we examine the influence of Coulomb collisions on the plasma potential profile in the downstream region. Figure 10 shows the variation of the plasma potential profile with collisionality. The collisionless potential profile is shown for comparison. Over a wide range of collisionality, the maximum variation of the plasma potential is less than one T_e . One concludes that the effect of ion-ion collisions on the plasma potential profile is weak compared to that caused by ion-neutral collisions. The reason behind this weak influence is that ion-ion collisions are energy- and momentum-conserving collisions. Scheuer and Emmert²⁰ reached the same conclusion in their study of the collisional plasma presheath.

Since Coulomb collisions do not cause large changes in the plasma potential profile, their effect on the parallel motion of the ions is also expected to be weak. Figure 11 shows the change in the parallel ion energy distribution at the sheath edge due to ion-ion collisions. In the collisionless case, the ion energy spectrum is necessarily the same as that at birth, but shifted to a higher energy, which corresponds to that gained in falling through the electrostatic potential. Note that as the collisionality increases, the peak energy slightly decreases (due to the reduction in the potential drop), while the width of the spectrum slightly increases.

Now, we examine the effect of Coulomb collisions on the ion perpendicular temperature $T_{\perp}$ and on the ion perpendicular velocity $v_{\perp}$. It is informative to start by looking at the spatial variation of $v_{\perp}$ in the absence of collisions. Figure 12 illustrates the spatial behavior of $v_{\perp}$ in a colli-

FIG. 11. The variation of the ion parallel energy spectrum at the sheath edge with collisionality. The dotted spectrum is computed at $X=0$. Argon plasma with ion-ion collisions only.

sionless argon plasma. The decrease in the peak and in the width of the spectrum is a result of the expansion of the magnetic-flux tube as X increases. Since the magnetic moment of the ion is conserved, as $|B|$ decreases $v_{\perp}$ should also decrease resulting in a low-velocity, narrow $v_{\perp}$ spectrum at the sheath edge. When ion-ion collisions are included, the $v_{\perp}$ spectrum at the sheath edge broadens with collisionality, and its peak shifts to a slightly higher velocity indicating a gain of energy in the perpendicular direction, as shown in Fig. 13. This is a result of diffusion in velocity space, which is a characteristic of Coulomb collisions. Figure 14 shows the variation of $T_{\perp i}/T_{\parallel i}$ ratio versus collisionality. The ratio $T_{\perp i}/T_{\parallel i}$ increases with collisionality, which indicates that energy is being transferred from the parallel to the perpendicular direction.

If ion-neutral collisions are also taken into account, the value of T_i may be considerably less than the 0.6 eV assumed in the simulation. Values of T_i below ~ 0.3 eV at neutral pressures above 1 mTorr were obtained in LIF experiments.⁷ Since the ion-ion mean free path is proportional to T_i^2 , Coulomb collisions will be even more important at low ion temperature. Therefore, considering ion-neutral and ion-ion collisions at the same time will enhance the effects of ion-ion collisions reported in this section.

FIG. 12. The spatial variation of the ion perpendicular velocity spectrum in a collisionless argon plasma.

FIG. 13. The variation of the ion perpendicular velocity spectrum with collisionality at the sheath edge. Argon plasma with ion-ion collisions only.

VI. EFFECT OF DOWNSTREAM IONIZATIONS

Downstream ionizations are produced either directly by hot electrons escaping from the source region, or by the tail of the bulk electron distribution function in the downstream region. In either case ions are created cold as a result of such ionizations. This will increase the ion density in the downstream region which will, consequently, reduce the electrostatic potential drop. To explore the effect of downstream ionizations we assumed uniform ionizations along the device axis. The creation of ions due to ionizing collisions is represented by a uniformly distributed ion source along the computational mesh. We also assumed that the integrated strength of this distributed source over the whole computational mesh is only 10% of the ion flux streaming out from the source region. Figure 15 shows the effect of downstream ionizations on both the potential profile and on the ion parallel energy distribution. The electrostatic potential variation in the downstream region decreases, and the ion energy distribution becomes more uniform as a result of ionizing collisions in the downstream region.

FIG. 14. The behavior of $T_{\perp i}/T_{\parallel i}$ with the normalized mean free path for ion-ion collisions in an argon plasma at sheath edge.

FIG. 15. Effect of downstream ionization on (a) the plasma potential profile, and (b) on the ion parallel energy spectrum at $X=0.4$. The case of no downstream ionization is labeled (I) while curves computed with uniform downstream ionization are labeled (II). Argon plasma at 0.3 mTorr.

VII. IMPLICATIONS OF THE RESULTS ON ECR PLASMA ETCHING

It was shown from the above results that charge exchange and elastic scattering collisions have a strong effect on ion dynamics in the downstream region of an ECR etching system. We now discuss some of the practical implications of these results on the etching process itself.

A basic role of the divergent magnetic field in the downstream region of a conventional ECR etching system is to extract the ions generated in the plasma chamber to the substrate stage. As discussed in Sec. IV A, the plasma potential profile is fairly flat at neutral pressures above 1 mTorr and, therefore, the impact ion energy is determined almost exclusively by the substrate's sheath drop. Including downstream ionizations will make this 1 mTorr pressure limit even lower, as discussed in Sec. VI. In another work, Hussein and Hitchon²¹ presented a simple analytic model that supports this behavior of the electrostatic potential with ion-neutral collisions in the presence of a divergent magnetic field. On the contrary, collisions increase the electrostatic potential drop in the absence of a magnetic field. This was shown analytically by Scheuer and Emmert, and numerically by Koch and Hitchon.²²

According to the above argument, and based on the results presented in Sec. IV A, the advantage of having a divergent magnetic field in the downstream region is lost at

neutral pressures above 1 mTorr (this pressure limit may vary depending on the conditions by which ions leave the source region and on the extent of downstream ionizations). Looking at the technology requirements for producing ultralarge-scale integrated circuits, one finds that etching uniformity over large wafers is essential. In addition, a highly anisotropic etching profile must be combined with high etching rates, objectives that are difficult to achieve simultaneously in a conventional ECR system.²³ The existence of the divergent magnetic field may actually make it more difficult to fulfill the above industrial requirements. The expansion of the magnetic-flux tube, as the plasma flows from the discharge chamber to the substrate, increases the plasma diameter and hence lowers the ion current density (which is directly related to etch rate) to the substrate. Also, the density of the radicals and other important chemical species is reduced due to the various recombination and relaxation processes that take place along the rather long flight path to the substrate.

The foregoing discussion suggests that a better process and a more efficient use of the plasma can be achieved by placing the substrate close to (or even inside) the discharge chamber, as demonstrated experimentally by Samukawa and co-workers.²³ In their work, Samukawa and co-workers produced an anisotropic etching profile with an etch rate of 1 $\mu\text{m}/\text{min}$ and a uniformity of $\pm 5\%$ on a 6 in. wafer by processing the wafer at the ECR position inside the discharge region. These etching characteristics are presumably a result of collimated ions, high ion current density, and uniform ion current at the ECR position.

VIII. SUMMARY

A numerical simulation of plasma flow in the downstream region of an ECR plasma etching reactor was presented. The work focused on exploring the effects of charge-exchange, elastic scattering, and ion-ion collisions on ion dynamics in the downstream region. As a result of ion-neutral (charge exchange and elastic scattering) collisions, the plasma potential drop across the downstream region and the peak ion energy decrease with neutral gas pressure in agreement with experimental measurements. The ion parallel energy spectrum was characterized by the existence of two peaks at low pressure. As pressure increases, the high-energy peak vanishes and a single low-energy peak dominates the distribution. The effect of ion-ion collisions on either the plasma potential or the ion parallel motion was found to be weak. Ion-ion collisions play an important role in transferring energy from the parallel direction, causing an increase in the transverse ion temperature, which may affect the anisotropy of the etching process. The simulation results showed that it is important (whenever $L > 10\lambda_{ii}$) to include ion-ion collisions in plasma models to account for the transverse heating of the ions.

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