JOURNAL OF APPLIED PHYSICS VOLUME 87, NUMBER 8 15 APRIL 2000

Calculation of ion energy distributions from radio frequency plasmas using a simplified kinetic approach

Martin Misakian[a] and Yicheng Wang
Electricity Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8113

(Received 23 November 1999; accepted for publication 18 January 2000)

Using an elementary kinetic approach, a procedure is described for calculating ion energy distributions (IEDs) from radio frequency (rf) plasmas. The calculated distributions, which are in the form of histograms, are used to fit experimental argon and CF_3^+ IEDs measured in a Gaseous Electronics Conference rf reactor modified to operate in a pulsed inductively coupled mode. Given the average plasma potential profile and its time dependence, the calculation incorporates a number of parameters used in more comprehensive treatments of the problem to determine the shape of the IED. The reverse calculation that determines the average potential profile, given an experimental IED, cannot be uniquely done, but some insights may be gained in some cases if a sufficient number of plasma related parameters are known, e.g., the shape and amplitude of the rf modulation. The results of the calculation indicate that argon ions forming the IEDs during the bright (H) mode come nearly exclusively from a presheath region that extends far into the interior of the plasma. The calculations also suggest that the CF_3^+ ions forming the IEDs observed during the dim (E) mode may preferentially come from near the ''edge'' of the bulk plasma. Possible significances of this difference are noted. © *2000 American Institute of Physics.* [S0021-8979(00)06908-5]

I. INTRODUCTION

Because ion bombardment plays a crucial role in etching discharges, considerable effort has been devoted to understanding how ion energy distributions (IEDs) are controlled by the plasma potential and associated electric field in the sheath region in various radio frequency (rf) plasmas. For example, Miller and Riley have investigated the physics of the plasma sheath using a semianalytic model,[1] and Hoekstra and Kushner[2] have studied IEDs in inductively coupled plasmas (ICPs) with chlorine-containing gas mixtures using a ''hybrid plasma equipment model'' linked with a ''plasma chemistry Monte Carlo simulation.'' Wild and Koidl[3] studied IEDs in capacitively coupled plasmas which exhibit multiple peaks. They explained the IED features by modeling the ion transport through rf modulated collisional sheaths. However, the shapes of observed IEDs are often explained only qualitatively. For example, Wang and Olthoff[4] attributed variations in IEDs observed in Ar, N_2, O_2, and Cl_2 plasmas to varying degrees of rf modulation across the ground sheath. This explanation is overly simplistic because the electric field in the presheath region may significantly influence the ion energy distributions.

Given the average potential profile and its time dependence, in this article we describe a procedure using an elementary kinetic model for calculating the shape of the IEDs from rf plasmas. The calculation leads to the construction of histograms that are used to fit experimentally determined IEDs. While the calculations incorporate some parameters included in more comprehensive treatments of the problem, e.g., the phase of the electric field, Maxwellian velocity distributions, charge exchange collisions, mean free paths, and points of origin of ions in the plasma,[2,3,5,6] the elementary approach may make the connection between these parameters and the IEDs measured more transparent. The experimental IEDs considered in this article are obtained from a 13.56 MHz argon plasma in a Gaseous Electronics Conference (GEC) rf reference reactor[7] modified to operate in a pulsed inductively coupled mode.[8,9] Given an experimentally determined IED, it may be possible to construct some features of the potential profile in the sheath and presheath[10] regions, although the uniqueness of the profile cannot be assured, as is discussed when considering a CF_3^+ IED.

II. EXPERIMENTAL APPARATUS

Plasmas were generated in a GEC rf reference reactor whose upper electrode was modified to house a five-turn planar rf-induction coil behind a quartz window to produce inductively coupled discharges.[8] The ion sampling arrangement is the same as that used to study inductively coupled plasmas generated in CF_4 under continuous excitation.[11] Ions are sampled through a 10 μm diam orifice in a 2.5 μm thick nickel foil that was spot welded into a small counterbore in the center of the bottom grounded electrode of the reactor. For IED measurements, the ions that pass through the orifice are accelerated and focused into a 45° electrostatic energy selector. After being selected according to their energy, the ions enter a quadrupole rf mass spectrometer where they are selected according to their mass-to-charge ratio and detected with an electron multiplier. The resolution of the electrostatic analyzer was fixed at a value of 1 eV, full width at half maximum, and the uncertainty of the energy scale is estimated to be less than ± 1 eV.

For pulsed operation of the reactor, the rf power to the inductive coil was supplied by a rf amplifier with its input

[a]Electronic mail: misakian@eeel.nist.gov

connected to a wave form synthesizer operating at 13.56 MHz. A master gate pulse generator with a variable pulse repetition rate and duty cycle was used to gate the rf output and to synchronize all time-resolved measurements. Time-resolved IED measurements were made by gating the digital ion counting pulses from the electron multiplier. The gating pulse, which could be varied in width, was synchronized to the master gate pulse generator through a variable digital delay generator.

When operated in the pulse mode, the plasma can exist in two states: a dim or E mode with characteristics of a capacitively coupled plasma, and a bright or H mode with characteristics of an inductively coupled plasma. When the rf energy is applied to the induction coil, the plasma for our conditions initially begins in the E mode and then undergoes a transition to the H mode.[9] Ion energy distributions measured during the E mode and H mode are considered for fitting using the model calculation method described in Sec. III.

III. KINETIC MODEL

We begin by considering an average electric potential in the sheath and presheath regions of the plasma that is a function of position. The approximation of one dimensional ion motion allows us to express the average potential as a function of the coordinate x, i.e., $V(x)$, and the negative gradient of $V(x)$ yields the average electric field, $E(x)$. Because the wavelength of the rf modulation (~ 22 m) is much greater than any relevant experimental dimension (<0.1 m), we make the assumptions that the electric field in our model is quasistatic[12] and that the time variation of the electric field and plasma potential can be incorporated as a multiplicative factor. That is,

$$V(x,T)=V(x)[1+\alpha \sin(\omega T+\Phi)], \tag{1}$$

and

$$E(x,T)=E(x)[1+\alpha \sin(\omega T+\Phi)], \tag{2}$$

where $\alpha V(x)$ is the amplitude of the rf modulation of the potential, ω is $2\pi f$ where f is the frequency, Φ is the phase of the potential or electric field when the ion enters the electric field, and T is the time at some instant (see below) during the time variation of the potential and electric field.

The force on an ion is

$$F=m\frac{dv}{dt}=qE(x)[1+\alpha \sin(\omega T+\Phi)], \tag{3}$$

where m and q are the mass and charge of the ion, respectively.

Equation (3) is solved in an approximate fashion using a step-by-step procedure during which the force is held constant as the ion moves a short prescribed distance toward the grounded bottom electrode of the GEC cell. The solution for the final velocity, v, after the ion travels some distance (taken below as Δx) is found by integrating Eq. (3), i.e.,

$$v=v_o+\frac{q}{m}E(x')[1+\alpha \sin(\omega T+\Phi)]t, \tag{4}$$

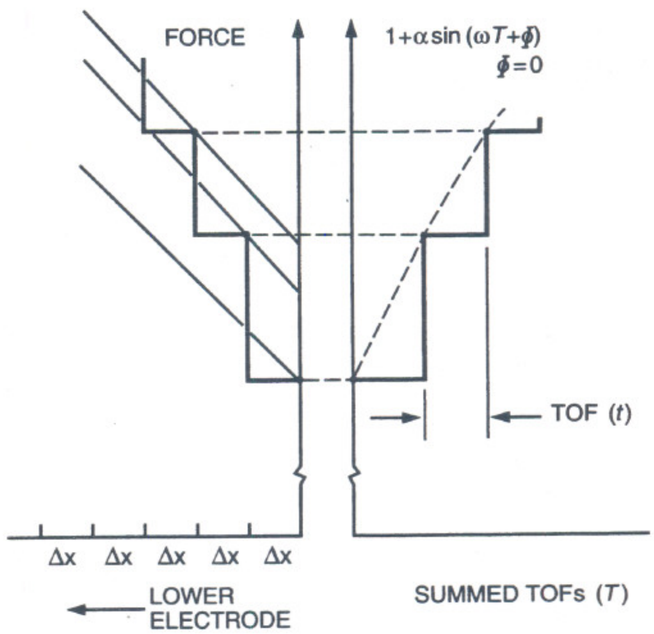

FIG. 1. Schematic view (not to scale) showing how the time dependent multiplicative factor in the equations is updated through the summation of TOFs, which together with the position of the ion (x) establishes the magnitude of the force for the next interval, Δx. A linear electric field is assumed here.

where v_o is the initial velocity, $E(x')[1+\alpha \sin(\omega T+\Phi)]$ is held constant, and t is the time of flight (TOF) with the initial value of t being taken as zero. T is the sum of the TOFs for traveling all of the earlier Δx intervals. A prime was added to the x value to indicate that it was held constant during the integration.

Noting that $v=dx/dt$ for the Δx interval under consideration, we can integrate both sides of Eq. (4) to obtain an expression for t as the ion travels the distance Δx,

$$\Delta x=v_o t+\frac{q}{m}E(x')[1+\alpha \sin(\omega T+\Phi)]\frac{t^2}{2}. \tag{5}$$

Equation (5) is a quadratic equation for t and is readily solved using the quadratic formula. The value of t is then used in Eq. (4) to determine v and this value of v becomes the initial velocity, v_o, for the next interval. The value of Δx is subtracted from the remaining distance to the grounded electrode to obtain the x' for the next interval and, as noted above, the value of t is added to the previous TOFs to obtain the new T. The "updated" product of $qE(x')[1+\alpha \sin(\omega T+\Phi)]$ becomes the force that is held constant for the next interval. Figure 1 illustrates schematically the step-by-step procedure. The process is repeated until the total distance traveled by the ion is equal to the assumed sheath/presheath width. The final velocity when the ion reaches the grounded bottom electrode is used to calculate the kinetic energy. By making Δx sufficiently small, it becomes possible to capture with adequate accuracy the magnitude of the changing force acting on the ion as it travels to the grounded electrode.

The model incorporates the effects of collisions, which are not included in the above equations, by considering the mean free path (mfp) of the ions during the calculation of the kinetic energies (see below). While we can anticipate that the mfp for argon ions will be mainly influenced by the large cross section for charge exchange, the mfp is used as a fitting parameter during the process of matching the calculated and measured IEDs. In gases where charge exchange or other collision processes that lead to the thermalization of the ion are not dominant, the approach described below would have to be modified because ions that travel to the grounded electrode are assumed to begin with thermal energies.

To construct histograms for fitting experimentally obtained IEDs, a computer program is used to calculate the kinetic energies of ions reaching the grounded electrode using the step-by-step procedure described above.

(1) The calculation assumes a given average electric potential profile (and associated electric field) that is amplitude modulated sinusoidally at a frequency of 13.56 MHz.
(2) Ions are created by electron impact ionization and charge exchange collisions.
(3) Ions initially have a range of thermal velocities given by the Maxwellian velocity distribution.
(4) Ions enter the field at a uniform rate in space and time for different phases, Φ, of the electric field.
(5) Ions originate uniformly from a range of starting points, X_o, where there exist both thermal ions and an electric field directed toward the grounded electrode.
(6) Because the mfp of an ion will change as its velocity increases, an average or ''effective'' mfp is assumed for the calculations (see below).
(7) Uniform temperature and pressure profiles are assumed to exist along the ion trajectory.
(8) The number of ions that arrive at the bottom plate are weighted by the function,

$$WT=\exp\left(-\frac{X_o}{L}\right)\exp\left(-\frac{mv_{\mathrm{T}}^2}{2k\mathrm{T}}\right), \tag{6}$$

where the first exponential is the mfp distribution with an average mfp value of L, and the second exponential is (within a constant) the Maxwellian velocity distribution, with k equal to the Boltzmann constant, T (not in italics) is the absolute temperature, and v_{T} is the thermal velocity of the ion as it begins its movement in the electric field toward the bottom electrode. For each ion arriving at the grounded electrode with energy in the interval E to $E+\Delta E$, an entry equal to the magnitude of WT is made in the appropriate energy bin to construct the IED histogram. The width of the energy bin used in the calculations described below is 0.2 eV.

IV. AVERAGE ELECTRIC POTENTIALS AND Ar^+ ION ENERGY DISTRIBUTIONS

To calculate the IED for argon ions from an argon plasma, we make use of the average plasma potential profile measurement by Miller *et al.*[8] in an inductively coupled continuous (not pulsed) argon plasma produced in a GEC rf reference cell and potential measurements 1.2 cm above the

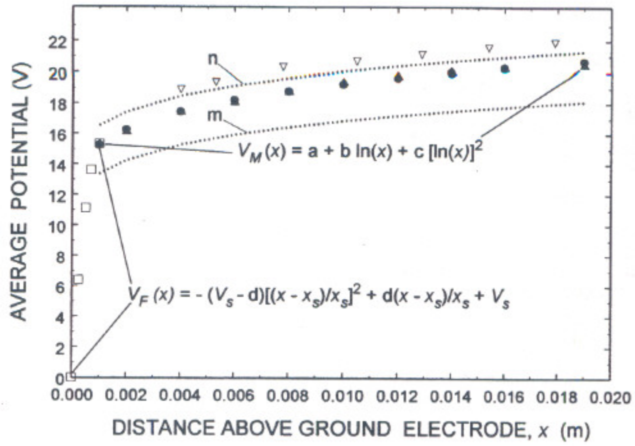

FIG. 2. Average potential profile after Miller *et al.* (Ref. 8) (▲). The triangles are fitted with the function $V_M(x)$, which is used to determine the electric field along the x axis between x_s and $x=0.019$ m. Predictions of $V_M(x)$ are indicated by closed circles (●). The open squares (□) represent several points predicted by $V_F(x)$, where $V_F(x)$ and the gradient of $V_F(x)$ were made to match the corresponding values for $V_M(x)$ at x_s. The open inverted triangles (▽) are the measurements of Schwabedissen *et al.* (Ref. 13), but they were not used in the calculations. Profiles m and n are used to calculate the IEDs in Fig. 3 and in the inset in Fig. 4, respectively.

grounded lower electrode in a GEC cell at the National Institute of Standards and Technology (NIST).[13] The power and pressure during the Miller *et al.* measurements were 150 W and 1.33 Pa (10 mTorr), respectively. The NIST measurements were performed as a function of pressure, but power information was not reported. Figure 2 shows a portion of the Miller *et al.* profile which extends from 0.1 cm above the grounded electrode (the lowest point measured) to a height of 1.9 cm.[14] The potential flattens at about 1.9 cm and argon ions in the plasma can from this point contribute to the calculated IEDs. The measurements of Miller *et al.* are fitted with a potential of the form,

$$V_M(x)=a+b\ln\left(\frac{x}{D}\right)+c\left[\ln\left(\frac{x}{D}\right)\right]^2, \tag{7}$$

where a, b, and c are equal to 32.77, 3.743, and 0.175, respectively, in units of volts. D is equal to 1 m and the values of x are expressed in units of meters.

The average potential between the bottom electrode and where it meets the Miller *et al.* potential is modeled with a potential of the form used by Fivaz *et al.*[15] for a linear electric field,

$$V_F(x)=-(V_s-d)\left(\frac{x-x_s}{x_s}\right)^2+d\frac{(x-x_s)}{x_s}+V_s, \tag{8}$$

where V_s is the potential value where $V_F(x)$ and $V_M(x)$ meet at a distance of x_s above the grounded electrode. Figure 2 shows the meeting point, x_s, as being equal to 0.1 cm but, as discussed later, better matches between the calculated and measured IEDs can be obtained by adjusting the value of x_s. The parameter d is used to match the gradient of $V_F(x)$ with that of the Miller *et al.* potential at $x=x_s$.[16] The negative gradients of $V_M(x)$ and $V_F(x)$ are the average electric fields that exert a force on the ions as they travel through the regions $x_s \leqslant x \leqslant 1.9$ and $0 \leqslant x < x_s$ cm respectively.

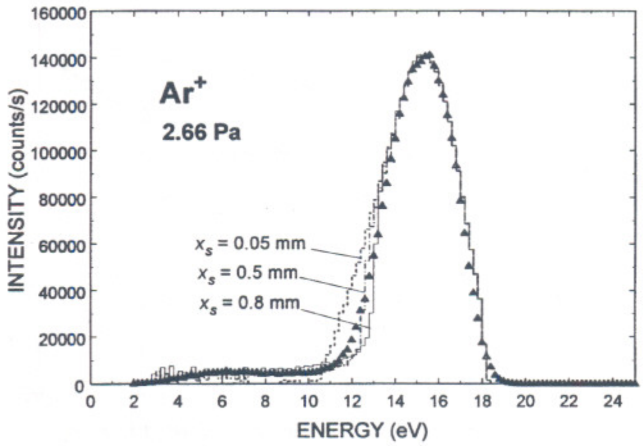

FIG. 3. Ar^+ IED measured during the bright mode (*H* mode) at 2.66 Pa (20 mTorr) and calculated energy distributions. The three histograms represent candidate matches between calculations and the measured IED assuming different values of x_s where $V_F(x)$ and $V_M(x)$ are joined. The peak heights of the histograms were made equal to that of the measured IED.

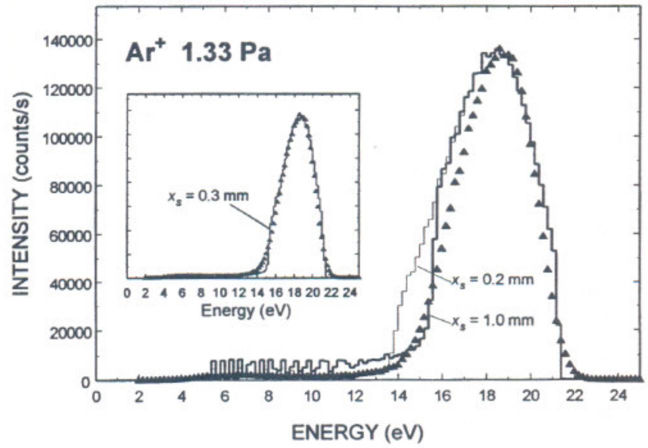

FIG. 4. Ar^+ IED measured during the bright mode at 1.33 Pa (10 mTorr) and two calculated energy distributions assuming different values of x_s. The peak heights of the histograms were made equal to that of the measured IED. The inset shows good agreement between the calculated and measured IEDs if a flatter average potential profile is used in the extended presheath region.

The open triangles in Fig. 2 show a portion of a potential profile measured in the NIST GEC reactor when the power and argon pressure were 84 W and 1.33 Pa, respectively.[13] These data were not considered for use in the model calculations because of their more limited range compared to the Miller *et al.* results.

Figure 3 shows an argon IED from an argon plasma in the NIST GEC rf cell measured during the bright mode of the discharge. During the measurements, the pressure was 2.66 Pa (20 mTorr) and the peak power[17] was 200 W. To perform the calculations, $V_M(x)$ was multiplied by a scaling factor of 0.876 to match the NIST potential measurements at $x=1.2\,\mathrm{cm}$ for the same pressure. After multiplying by the scaling factor, the values of a, b, and c [Eq. (7)] become 28.70, 3.278, and 0.1528, respectively (Fig. 2, profile m). The same scaling factor was also applied to $V_F(x)$. The significance of using a multiplicative scaling factor and not an additive constant to $V_M(x)$ is discussed later. Figure 3 also shows the results of three calculations assuming different values of x_s where $V_M(x)$ and $V_F(x)$ are joined. Assuming $x_s=0.05\,\mathrm{mm}$ ($d=0.251$) leads to the elimination of most ions in the low energy tail of the IED. The results for $x_s=0.8\,\mathrm{mm}$ ($d=1.098$) and $x_s=0.5\,\mathrm{mm}$ ($d=0.955$) are similar although, while not obvious from Fig. 3, a better match is obtained for the low energy tail when $x_s=0.8\,\mathrm{mm}$. A slightly improved match is obtained with the main portion of the IED ($>12\,\mathrm{eV}$) by using $x_s=0.5\,\mathrm{mm}$.

The IED calculations assume an average mfp (L) of 0.52 cm, a temperature of 600 K,[18] and ions that originate from 1.9 to roughly 0.01 cm above the grounded electrode contribute to the energy distribution. The value of Δx was 9.5 $\times 10^{-5}$ cm and the separation in X_o values was 26 μm for most of the calculation, although the main features of the IED (between ~ 12 and 18.1 eV) could be determined with values twice as large.[19] The calculation takes into account values of the phase, Φ, ranging from 0° to 358° in 2° steps, and assumes the amplitude of the rf oscillations of the plasma potential, αV (1.9 cm), is equal to 0.75 V which is similar to a previously reported amplitude in an argon plasma.[20] The calculated histogram is not highly sensitive to small changes in the value of $\alpha\ V$ (1.9 cm). The thermal velocities, v_T, considered for the weighting function, *WT*, increased from zero in 100 m/s steps to a value for which *WT* was less than 0.0015.

Assuming that the gas pressure measurement accurately reflects the pressure over the path taken by the ion, we use the approximate relation between the mfp, L, the gas density, n, and the cross section,[21] σ, i.e., $L\approx 1/n\sigma$, to obtain an estimate of the average cross section. For the given conditions, $\sigma\approx 5.9\times 10^{-15}\,\mathrm{cm}^2$, which is consistent with an $Ar+Ar^+$ charge-transfer cross section, but near the upper limit for the range of published cross section values, i.e., between $\sim 6\times 10^{-15}$ and $\sim 3.5\times 10^{-15}\,\mathrm{cm}^2$ for ion kinetic energies of $1-\sim 20\,\mathrm{eV}$.[22]

Figure 4 shows an argon IED recorded in the NIST GEC reactor during the bright mode at a pressure of 1.33 Pa (10 mTorr). For this case, the NIST potential measurement at $x=1.2\,\mathrm{cm}$ above the grounded electrode for the same pressure suggested that the potential profile [Eqs. (7) and (8)] be scaled upward by a factor of about 1.045. This leads to a potential at $x=1.9\,\mathrm{cm}$ of 21.6 V, which in turn leads to a maximum ion kinetic energy near 21.6 eV, ignoring the instrumental spreading of the IED. The maximum kinetic energy in Fig. 4 is near 21.3 eV, which is slightly lower. Therefore, to fit the IED in Fig. 4, the scaling factor was chosen so that the maximum kinetic energy from the calculation would match the IED data, i.e., the scaling factor was made 1.03, raising the average potential at $x=1.9\,\mathrm{cm}$ to 21.3 V. For this case, the values of a, b, and c are 33.76, 3.855, and 0.1797, respectively.

Figure 4 also shows two calculated IEDs assuming x_s values of 0.2 mm ($d=0.793$) and 1.0 mm ($d=1.332$). While not clear from Fig. 4, the histogram for $x_s=0.2\,\mathrm{mm}$ predicts a low intensity of ions in the low energy tail,