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Signatures of the Bohm and sheath velocities in minority-light-ion energy distributions

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The energy distributions of light minority ions impinging on the walls of a radiofrequency plasma are obtained numerically by integrating trajectories in a self-consistent electric field. The distributions are found to contain features which can be directly related to the Bohm and sheath velocities. The genesis of these features is considered and a comparison is made to experimentally determined distributions in a mixture of argon and 8% helium.

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The energy distributions of ions incident on the bounding surfaces of low pressure radiofrequency (rf) driven plasmas have been subjected to intense study since the ion flux is an important agent in many plasma processing applications. In the most thoroughly studied cases, the ion spectra exhibit features due both to the rf modulation of the electric field in the plasma sheath and to the collisions which the ions undergo while they are accelerated during their passage through the sheath. Since these low temperature plasmas are weakly ionized, the most abundant ion species is frequently the singly charged ion of the background gas atom or molecule and resonant charge exchange strongly influences the ion motion through the sheath [1]. When resonant charge exchange is not important, which may occur in the case of minority species [2] or at sufficiently low pressure, the distributions are found to have two peaks and are hence called "bimodal" or "saddle" distributions [3].

Analytic expressions for the shape of the distributions as well as the energy splitting between the peaks are available [4,3], and can even include ponderomotive effects [5], but they are restricted to heavy ions or wide sheaths for which the ion transit time τ_i through the sheath is much longer than the rf period $2\pi/\omega_{\rm rf}$, and often also to simple model (non-self-consistent) electric fields. For the more general case of arbitrary transit times and when the effects of collisions are to be included the distributions are obtained by numerical integration of the ion trajectories through the sheath, most commonly in simple model or analytically derived fields [6–8]. Ion distributions are also obtained in self-consistent kinetic simulations of rf plasmas [9,10].

In this paper we examine the distributions of light minority ions in rf plasmas under conditions where collisions can either be neglected or do not interfere with the measurement of the basic saddle structure. Light minority ions are of considerable practical interest since they are common in laboratory and processing plasmas. Even a small amount of residual water vapor in an argon plasma can lead to the production of measurable fluxes of H_3^+ ions [11]. H^+ and H_2^+ can be produced in plasmas burning in technologically important gases such as SiH_4, CH_4, CHF_3 and in mixtures of etchant gases with hydrogen. Another light ion often found in processing plasmas is He^+, since helium is used to improve the thermal contact between the wafer being processed and the temperature controlled holding chuck. In many cases the light ion density is only a few percent of the total ion density and the structure of the rf sheath is determined by the flux of the heavy ions. Light ions can then have short transit times—between 0.5 and 2 rf periods—and measurement of their distributions is attractive as a diagnostic of the sheath structure since sensitivity to variations in the electric field is greatly enhanced.

In order to demonstrate some of the possibilities of light ions as a sheath diagnostic, we obtain light ion distributions in a collisionless sheath by numerical integration of ion trajectories through the self-consistent sheath field given by Lieberman [12]. This is characterized by the movement of a sheath edge or electron density front—assumed to be steplike in the model—which separates two regions of zero field behind the edge where electrons balance the ion space charge and the field given by

$$E = \frac{e}{\epsilon_0} \int_{s(t)}^{x} n_i(\xi) d\xi \qquad (1)$$

ahead of the sheath edge whose position is given by

$$s(t) = s_0 \left[(1 - \cos\theta) + \frac{H}{8} \left(\frac{3}{2} \sin\theta + \frac{11}{18} \sin 3\theta - 3\theta \cos\theta - \frac{\theta}{3} \cos 3\theta \right) \right] \qquad (2)$$

with $\theta = \omega_{\rm rf} t$, $s_0 = J_{\rm rf}/(e\omega_{\rm rf} n_0)$, $J_{\rm rf}$ and $\omega_{\rm rf}$ the amplitude of the sinusoidal rf current and the angular rf frequency, respectively, and $H = (1/\pi)(s_0/\lambda_D)^2$, where λ_D is the electron Debye length at the edge of the sheath region where the electron density is n_0.

The electric field in the sheath cannot be written out explicitly and the simulation starts with a choice of the input parameters which are used to calculate the field in the complete range of x and θ values and to fill a lookup table. Electric field values for the trajectory integration are interpolated from the lookup table. We are considering plasmas with a single dominant ion species and assume in this work that the light minority ions have a low enough concentration so that the density of light ions in the sheath can be neglected in the electric field evaluation. The general approach is essentially identical to that used by Barnes *et al.* [8], although we leave the rf frequency fixed at 13.56 MHz and vary only n_0, $J_{\rm rf}$, and the electron temperature T_e. The short transit times led us to adopt an adaptive step integration since much of the cycle is taken up by drift through the field free regions, yet high fields near the wall require short time steps for adequate accuracy. Initial entry phases are picked randomly within the rf cycle and the ions enter the sheath with the Bohm velocity $u_b = (eT_e/m_i)^{1/2}$, where m_i is the ion mass. Typically 10^5 ions are used for each distribution.

The modulation of the electric field in the sheath leads to the well known variation of the final ion energy with its entry phase. Since the final energy has a continuous dependence of the initial phase in a collisionless sheath, it follows that peaks in the energy distribution will occur at the two special phases which results in maximum and minimum energy. The distribution for He$^+$ with $n_0 = 9\times10^{15}$ m^{-3}, $T_e = 1.9$ eV, and $J_{\rm rf} = 38$ Am^{-2} [13] is shown in Fig. 1. Remarkably, it is not simple. Although the two peaks at the energy extremes dominate, extra structure, consisting of an asymmetric peak at about 58 eV, is evident between them. We now consider the origin and significance of this peak.

Reflecting on the ion entry phase, we may note that in addition to the two special entry phases which result in minimum and maximum exit energies, there is another special entry phase in the rf cycle. Since the ions enter the sheath at the Bohm velocity, an entry phase exists for which the trajectory is a tangent to the curve defining the instantaneous position of the sheath. This trajectory is shown as the dashed line in Fig. 2, where trajectories just ahead and just after the tangent trajectory are also shown. It can be understood how a peak forms at this entry phase by considering what happens to ions which enter just before and just after the tangent phase. Ions that enter just ahead experience a slight push as the sheath front sweeps over them. They then drift through the field free region and are finally swept out to the wall during the following rf cycle. Those further ahead of the tangent phase gain more energy so that the trajectories are dispersed or "fan out" ahead of this phase. In contrast, the ions entering after the tangent phase experience no impulse from the field and their trajectories remain parallel until they enter the electric field during the following sheath expansion period. If the density of trajectories is considered, there is a drop before the tangent phase which can result in a step structure in the energy distribution. This drop will appear on the high energy side in the spectrum. Finally, those ions which drift through the field free region with parallel trajectories (constant density of trajectories) experience bunching when they enter the expanding sheath field (those with later entry phases experiencing a higher field) so that an actual peak in the distribution forms. Both the position and shape of this peak are sensitive to the Bohm velocity as is demonstrated in Fig. 3, where the distributions of ions with different masses are shown for otherwise identical conditions.

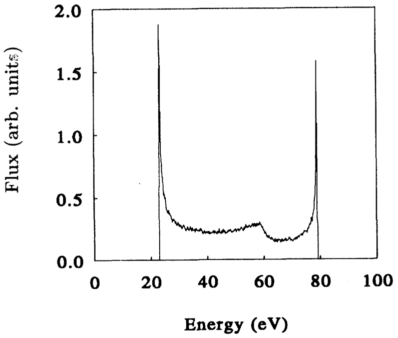

FIG. 1. Simulated helium ion energy distribution.

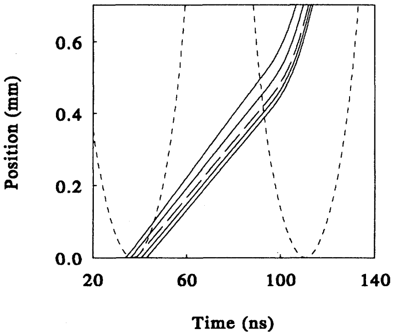

FIG. 2. Ion trajectories near the tangent trajectory which is shown dashed. The movement of the sheath front is shown as the dotted line. Entry phases are evenly spaced by 0.2 radians and only about one-half of the sheath is shown.

The consideration of special trajectories leads to the identification of another possibility where the ion trajectory approaches a tangent to the sheath position. The simulations indicate that dispersal of trajectories occurs when fast ions move near the instantaneous sheath edge with velocities closely matching the velocity of the electron front as it approaches the wall. Only a small field is present and the trajectories of ions entering the field free

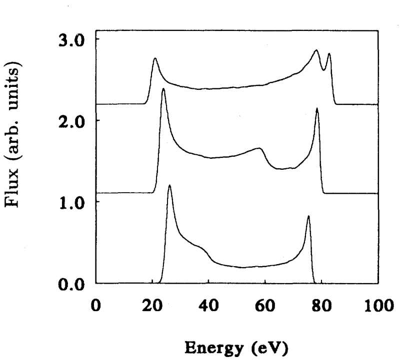

FIG. 3. Energy distributions for $m_i = 3m_p$ (top), $m_i = 4m_p$ (middle), and $m_i = 5m_p$ (bottom). Sheath parameters are constant and the distributions have been convoluted with a 0.9 eV Gaussian profile, to show the effect of limited analyzer resolution, and displaced vertically to enhance clarity.

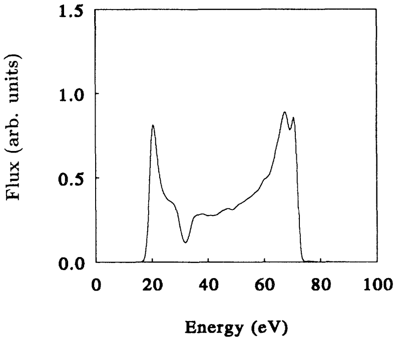

FIG. 4. Ion energy distribution for $m_i = 2.5m_p$ convoluted with a 0.9 eV Gaussian profile.

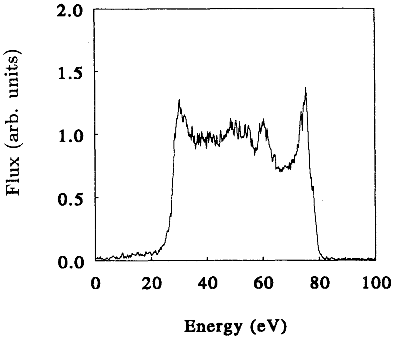

FIG. 5. He^+ energy distribution in an argon plasma at 25 mTorr and 50 W input power.

region are sensitive to the phase at which they cross the position of the sheath edge. The situation is completely analogous to the dispersal of trajectories discussed above in connection with the Bohm velocity, except in this case dispersal effectively occurs in the opposite direction since ions with later entry phases cross the sheath edge earlier.

For helium ions under the conditions given above this is a very slight effect, however, sufficiently light ions are able to track the sheath edge at the maximum sheath velocity. The ion trajectory becomes unstable if the velocity of the ions reaching the wall near $\theta = \pi$ [cf Eq. (2)] is close to the maximum sheath velocity. The instability is a consequence of small perturbations which are caused by numerical errors in the simulation, but field fluctuations would produce a similar effect in a laboratory plasma. Parametric studies confirm that an instability occurs for lighter ions which can track the edge longer, at lower field values, and are therefore sensitive to smaller perturbations. An example of the effect of unstable trajectories on the distribution is evident in the valley at 30 eV in Fig. 4, where the distribution of ions with $m_i = 2.5m_p$ is shown for a sheath with $n_0 = 5 \times 10^{15}$ m^{-3}, $J_{\mathrm{rf}} = 30$ Am^{-2}, and $T_e = 3$ eV. The fractional ion mass is used purely for demonstration purposes but we note that certain multiply charged ions are dynamically equivalent to ions of fractional mass.

We are led to the conclusion that the light ion distributions can contain the signatures of perhaps the two most important velocities associated with the rf sheath: the Bohm velocity and the sheath velocity. The shape of the additional peak, or step, may provide some information on the velocity distribution of the ions entering the sheath and, for very light ions, the valley can provide an estimate of the maximum sheath velocity. There is yet further fine structure in the distribution and detailed analysis of the simulation results indicates that bunching —leading to formation of a small peak—occurs for ions which reach the wall near the phase where the electric field is rising most rapidly, i.e., at the maximum displacement current, while debunching—giving a small valley—occurs near the wall when the field is dropping most rapidly.

The question naturally arises whether the structures identified in the simulation can be observed experimentally. The energy distribution of He^+ ions in an argon plasma at 25 mTorr is shown in Fig. 5 for a helium partial pressure of 8%. The data were taken at the grounded electrode of a parallel-plate rf discharge equipped with a mass-resolved ion energy analyzer as described by Snijkers *et al.* [11]. Extra structure appears between the two extreme energy peaks. Comparison with Fig. 1 suggests that the peak at 60 eV is the expected signature of the Bohm velocity. Exploratory parametric studies show that the small dip at 57 eV is unlikely to be due to the unstable trajectories discussed above and it may be associated with the debunching of trajectories which occurs as the displacement current reaches its most negative value.

It should be noted that the field used in the simulations is very simple and tight agreement between simulation and experiment, particularly in the peak shapes and heights, is not to be expected. The differences in detail between the experimental and simulated distributions can be regarded as further evidence that the light ion spectra contain valuable information on the structure of the sheath field. Comparisons of the present results to simulations using electric fields obtained by particle-in-cell techniques and including collisions will be presented in a future publication [14].

It has been shown by consideration of simulated and experimentally determined energy distributions that the Bohm velocity and the sheath velocity can give rise to identifiable features at definite ion energies. The mechanism responsible in both cases is the dispersion of trajectories near the moving sheath edge. The study of light minority ions, such as He^+ in argon plasmas, leads to the identification of experimental support for the existence of the Bohm velocity in the sense of a distinct velocity of the majority of the ions entering the sheath from the presheath. It can also provide information on the structure of the electric field in an rf plasma sheath.

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