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RECONSTRUCTION OF THE TIME-AVERAGED SHEATH POTENTIAL PROFILE IN AN ARGON RF PLASMA USING THE ION ENERGY DISTRIBUTION

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Short title: Reconstruction of the sheath potential profile

Abstract. Charge-exchange collisions and radio-frequency excitation combine to give peaks in the ion energy distribution measured at the ground electrode of an argon plasma in a capacitive reactor. These peaks are used as a diagnostic to reconstruct the profile of the time-averaged potential in the sheath. Particle-In-Cell simulations show that the method is accurate. The method is applied to investigate the sheath thickness as a function of excitation frequency at constant plasma power. The time-averaged potential is found to be parabolic in both experimental measurements and numerical simulation.

1. Introduction

The potential profile for a collisional sheath influences the energy distribution of ions impinging on the substrate of a plasma reactor. In practice, however, the sheath electric field in a radio-frequency (RF) discharge is difficult to measure because the sheath is thin (a few mm) and easily perturbed by probes. Previous techniques in RF plasmas include electron beam diagnostics [1] or the Stark effect in laser-induced fluorescence experiments [2], both of which require line-of-sight access through the sheath. In this work, the ions themselves are used as probes for the sheath potential profile by measuring the ion flux energy distribution with a mass spectrometer mounted in the ground electrode.

The interaction of the RF voltage and charge exchange collisions in the sheath gives rise to peaks in the ion energy distribution at the electrodes. Wild and Koidl [3] derived an analytical description for the ion energy distribution in a highly asymmetric discharge. Their model assumes a power law for the ion density profile in the sheath and has several free parameters which give an accurate fit to their experimental data. In what follows, we establish a simple explicit method to reconstruct directly the time-averaged sheath potential profile using the peak energies in the ion energy spectrum. The method is applicable to other plasmas in which charge-exchange collisions occur. A Particle-In-Cell and Monte-Carlo simulation code [4] is used to test and validate the method presented for reconstructing the potential. Finally, experimental measurements and numerical simulation are compared by using the technique to estimate the sheath width dependence on RF excitation frequency.

2. Description of the experiment and numerical simulation

The experimental apparatus is a parallel-plate capacitive reactor [5] comprising two cylindrical electrodes 130 mm diameter with a 25 mm electrode gap. The argon pressure was 0.1 Torr and the capacitively-coupled excitation frequency was varied from 13.56 to 42 MHz for plasma powers in the range 1 to 10 W. The power in the plasma was estimated by a subtractive method [6] using a voltage probe mounted on the underside of the RF electrode [7]. A Hiden Analytical

Limited [8] Plasma Monitor HAL-EQP 500 measured the mass and energy of ions impinging on the ground electrode at the electrode axis (Fig. 1). The ions entered the monitor first through a 5 mm diameter orifice in the ground electrode and then through a 100 μm aperture in the negatively-biased (-50 V) extractor head. The method is applicable to electrode areas of arbitrary asymmetry, but since the experimental data were to be compared with a 1D numerical simulation along the electrode axis, it was necessary to symmetrize the effective areas of the ground and RF electrodes. This was achieved by confining the plasma within concentric metal screens, as shown in Fig. 1, to obtain approximately zero self-bias of the RF electrode (≤ 5 % of the peak-to-peak RF voltage): the plasma potential with respect to each electrode is then of equal amplitude and in anti-phase [9]. The discharge was thus considered to be symmetrized.

The code XPDP1 [4] is a 1D Particle-In-Cell (PIC) and Monte-Carlo collision code applicable to a symmetric plasma geometry. It provides a fully kinetic representation for plasma ions and electrons. Cross-section models for ion-neutral and electron-neutral collisions in an argon plasma simulate charge exchange collisions, ionization, excitation and elastic scattering. The argon gas is treated as a uniform, static background. This code was implemented on a parallel computer called MUSIC [10], allowing very long simulations (10^3 RF periods) of the experiment. The RF electrode voltage in the simulation was taken from the experimentally-measured applied voltage corresponding to the required plasma conditions to be simulated.

3. Results and Description of the Method

3.1 Ion energy spectra

The argon ion flux energy distribution in figure 2(*a*) is obtained from the PIC simulation. This is compared with the mass spectrometer experimental measurement in figure 2(*b*) for the same nominal plasma parameters (i.e. the same reactor geometry, argon pressure and applied RF voltage). Although the peaks do not match in detail, the simulated and experimental spectra have the same general structure; the difference will be further comented upon in section 3.5. The dispersion of the Ar^+ ion energy distribution is due to symmetric resonant charge exchange collisions with the background neutral gas which effectively reduce the ion velocities to zero after each collision [11] as they cross the sheath potential on the way to the electrode.

The excitation frequencies used here are much higher than the sheath transit frequency for the ions, and therefore their average motion towards the electrodes depends on the time-averaged sheath electric fields [3,9]. The ion flux energy distribution of Ar^+ ions can thus be considered as a superposition of two components: i) an energy spectrum corresponding to ion collisional drift across a time-averaged (stationary) sheath electric field; and ii) a peak-structured energy spectrum due to the combined effect of the oscillating RF field and charge exchange collisions [3]. According to the model of Davis and Vanderslice [12], the ion flux energy distribution $\Gamma(E)$ across a stationary sheath electric field is given by:

$$\Gamma(E) = \frac{x_s}{2\lambda}\left(1 - E/V_s\right)^{-1/2} \exp\left(-\frac{x_s}{\lambda}\left[1-\left(1 - E/V_s\right)^{1/2}\right]\right) \qquad (1)$$

where x_s / λ is the ratio of sheath width to mean-free-path for charge exchange, E is the ion energy (in eV) and V_s (V) is the potential drop across the sheath. This sheath model assumes no ionization and a linear electric field in the sheath region - the assumption of linearity will be commented upon in section 3.4. A fit for parameter x_s / λ of equation (1) to the measured ion spectrum is shown on figure 2: the ion spectrum is well reproduced by this model, except for the peaked structure.

Also shown in Fig. 2(*b*) is the energy distribution of ArH^+ ions which are formed by Ar^+ reacting with hydrogen from residual water in the reactor. ArH^+ ions do not suffer symmetric resonant charge exchange collisions because the equivalent neutral does not exist. They therefore cross the sheath with negligible probability of inelastic collisions and their energy distribution at the electrode is a single peak with energy equal to the time-averaged sheath potential, providing a useful experimental measurement of V_s.

3.2 Origin of the peaks

The electron plasma frequency is much higher than the excitation frequency and they follow the time variation of the RF field. Within each RF period there is a short time interval during which the electric field disappears throughout the sheath. This is necessary for electrons to reach the electrode since the time-averaged discharge current is zero with capacitive coupling. Ions created by charge exchange during this time interval accumulate at zero velocity. Subsequently, as the electric field reappears, these ions drift as a bunch towards the electrode. Bunches relative to successive periods can be seen on figure 3, which represents a snapshot of ion phase space in the sheath given by the PIC simulation. When the field vanishes again at a later time, the bunched ions drift at constant velocity and accumulate on the electrode at approximately the same energy and time. This gives rise to a peak in the spectrum seen on Figure 2. This phenomena was described in detail by Wild and Koidl [3], who also show that the higher energy peaks split and tend to overlap. Experimentally, the peak structure is most clearly visible for high power, low frequency discharges.

3.3 Piecewise linear reconstruction of the sheath potential profile

Let us denote E_n (n=1,2,...) the increasing energies (in eV) of the successive peaks in the spectrum. On the basis of the above explanation, one can assert that the ions forming the energy peak E_n started at rest from a point x_n in the sheath where the time-averaged potential $V(x_n)$ equals E_n. The time taken for these ions to reach the electrode is nT, where T is the RF period. The problem of recovering the potential in the sheath thus reduces to determining these initial positions x_n.

In a first approach, we approximate the potential by a piecewise linear function, linear on each interval $[x_j, x_{j-1}]$. Let us consider an ion which will finally contribute to peak n. During the time interval Δt_j where the ion crosses the interval $[x_j,x_{j-1}]$, the gain in momentum Δp can be written, using energy conservation:

$$\Delta p = -\frac{E_j - E_{j-1}}{x_j - x_{j-1}} \Delta t_j = \sqrt{2m}\left(\sqrt{E_n - E_j} - \sqrt{E_n - E_{j-1}}\right) \qquad (2)$$

where m is the ion mass. Summing the total time, $nT = \sum_{i=1}^{n} \Delta t_j$, for the ion to reach the electrode from x_n, one obtains the following iterative relation:

$$x_n = x_{n-1} + \sqrt{E_n - E_{n-1}}\left[\frac{nT}{\sqrt{2m_i}} - \sum_{j=1}^{n-1} \frac{x_j - x_{j-1}}{E_j - E_{j-1}}\left(\sqrt{E_n - E_{j-1}} - \sqrt{E_n - E_j}\right)\right] \qquad (3)$$

where $x_o = 0$ is the electrode position. When all the positions x_n for the peaks E_n have been determined, the piecewise linear potential is extrapolated from the highest energy peak up to the sheath potential V_s, which is given by the maximum energy of the Ar^+ energy spectrum, or the ArH^+ peak energy. The corresponding abscissa x_s for the potential V_s determines the sheath width.

The validity and accuracy of this method can be checked with PIC simulations which provide both the ion energy spectrum at the electrodes and the corresponding time-averaged potential in the plasma. The potential profile reconstructed from the peaks in the simulated energy spectrum using the linear piecewise method is compared to the actual simulated potential profile in figure 4. The method is precise to within a few percent.

3.4 Parabolic reconstruction of the sheath potential profile

For the range of plasma parameters investigated, both for simulation and experiment, a parabolic fit for the sheath potential profile is found to be a good approximation to the reconstructed piecewise linear potential. For this reason, we consider a second approach in which a parabolic form is assumed for the potential:

$$V(x) = -a \left(\frac{x - x_s}{x_s}\right)^2 + b \left(\frac{x - x_s}{x_s}\right) + V_s \qquad (4)$$

where $-b / x_s$ is the small but non-zero electric field at the sheath/plasma boundary [11], and

$a + b = V_s$. From the conservation of energy in this potential, an ion starting from rest at x_n reaches the electrode with energy E_n in time nT where

$$nT = \int_0^{x_n} \frac{dx}{\sqrt{2\left(E_n - V(x)\right)/m}} \tag{5}$$

An evaluation of the sheath width $x_s^{(n)}$ corresponding to each peak n is then given by:

$$x_s^{(n)} = \sqrt{\frac{2a}{m}}\, n\, T \left[\operatorname{arccosh} \frac{1 + b/2a}{\sqrt{(V_s - E_n)/a + b^2/4a^2}}\right]^{-1} \tag{6}$$

A minimum in the variance of the set $\{x_s^{(n)}\}$ is found when b is varied. An estimation of the sheath width is then given by the average of the set $\{x_s^{(n)}\}$ for this minimum variance condition. The parabolic reconstruction corresponds closely to the linear piecewise reconstruction and the simulated potential profile as shown in figure 4.

It is important to associate the right number of periods to the peaks used, i.e. the peak numbering must be correct. The first peak may be missed because it can be weak compared to the strongly-varying background at low energy (see Fig. 2). In this case, the variance of the x_s values is large. By allowing for a shift in the peak numbering, a set of approximately equal x_s values confirms the correct peak identification. The reconstruction does not change significantly if the highest energy peaks are not used.

A parabolic potential profile implies a linear electric field and constant charge density throughout the sheath. The good fit to the data in figures 2(*a*) and (*b*) of the expression of Davis and Vanderslice [12] is therefore consistent with the linear electric field assumption in their model. However, the ion density in the sheath is not constant: it must decrease towards the electrode because the ion flux is constant (negligible ionisation) and the average ion velocity increases [11]. The PIC simulation in figure 4 shows in fact that the time-averaged electron density profile in the sheath region compensates the spatial variation in ion density so as to produce a constant total charge density.

3.5 Comparison of experiment and numerical simulation

Numerical simulation and experiment give similar results for the potential profile and sheath width as shown in figure 5. The experimental value is found to be systematically smaller than the width given by simulation. This may be due to the mass spectrometer extraction voltage locally perturbing the sheath: the ground equipotential surface is estimated to be displaced by 0.2 to 0.4 mm into the sheath region, as calculated by a 2D electrostatic potential solver. This perturbation would also account for the difference in peak structure in figures 2(*a*) and (*b*).

The method was applied to estimate the sheath width as a function of excitation frequency at constant plasma power in figure 6. The observed trend of thinner sheaths at higher frequencies is confirmed by other studies [13-15] and by optical measurements. Finally, the sheath width estimated from the Davis and Vanderslice [12] fit (Eq. (1)) to the experimental ion flux energy distribution is compared with the reconstruction method in Table 1, showing good agreement.

The reconstructed potential can be used to give more information about the plasma characteristics. For example, at the electrode surface, since the electron density is much smaller than the ion density, the second derivative of this potential gives the ion charge density n_i. The average ion velocity $\langle v_i \rangle$ can be evaluated from the energy spectrum at the electrode, and the absolute ion flux at the electrode is then given by $n_i \langle v_i \rangle$. This flux evaluation method is of interest for experiments because the integral of the experimental ion energy distribution does not give a reliable absolute flux since the spectrometer extraction efficiency is not accurately known.

4. Conclusions

A method for determining the profile of the time-averaged sheath potential by energy-resolved mass spectrometry in argon RF discharges has been presented, in which the ions themselves are used as probes for the sheath potential profile. Particle-In-Cell simulations show that the reconstruction is accurate if the peaks in the ion energy spectrum at the electrode can be numbered unambiguously. The reconstructed potential profile is found to be parabolic, corresponding to a time-averaged linear electric field in the sheath region. Numerical simulation and experiment show good agreement for the ion energy distribution, the parabolic sheath potential profile, and the sheath width estimations. The method is employed to show the reduction in sheath width with increasing RF excitation frequency.

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Table

Table 1: Comparison of experimentally-measured sheath widths estimated using the reconstruction method (Eq. (6)) and the Davis and Vanderslice model (Eq. (1)) with 0.5 mm mean-free-path for charge exchange collisions (gas density 3.5 10^{21} m^{-3}, argon charge exchange cross-section 5.7 10^{-19} m^{-2}). The corresponding RF plasma powers are indicated in parentheses.

Frequency (MHz)	sheath width (mm) using Eq. (1)	reconstructed sheath width (mm) using Eq. (6)
25 (7 W)	3.3	3.2
30 (7 W)	3.0	2.9
42 (7 W)	2.1	1.5
13.56 (3 W)	4.5	4.5
18.5 (3 W)	3.7	4.1
25 (3 W)	2.8	3.0
30 (3 W)	2.6	2.4

Figure captions

Figure 1: Schematic of the cylindrical electrodes, concentric screens, mass spectrometer orifice and extraction electrode. The RF screen height H was adjusted to obtain approximately zero self-bias of the RF electrode as measured by the voltage probe.

Figure 2: Energy distribution of the argon ion flux at the ground electrode: (*a*) by Particle-In-Cell simulation; and (*b*) as measured experimentally. The dashed curves show a non-linear least-squares fit using Eq. (1) to each energy distribution, for which $x_s / \lambda = 5.8$ and 5.5 for (*a*) and (*b*) respectively. The peaks are clearly shown by the difference of the energy distribution and the corresponding fitted curve in (*a*) and (*b*). The measured ArH^+ energy spectrum (multiplied by a factor 30) is also shown in (*b*). Excitation frequency 25 MHz, for 3 W power in the plasma.

Figure 3: Snapshot of the ion phase space in the sheath, as given by a PIC simulation. Each dot represents an ion. The ground electrode is on the left, the plasma bulk on the right. The arrows indicate, in ascending order, the ion bunches created approximately 0, 1, 2 and 3 RF periods before the snapshot.

Figure 4: Time-averaged profiles from PIC simulation. The potential profile given by the simulation is shown by the continuous curve. The linear piecewise reconstruction from the peaks in the simulated ion energy spectrum is represented by the square dots. The parabolic reconstruction is shown by the dashed curve. The ion and electron density profiles n_i and n_e are commented upon in section 3.4. Excitation frequency 25 MHz, for 3 W power in the plasma.

Figure 5: Experimental potential given by linear (points) and parabolic (full line) reconstructions, in comparison with the potential from PIC simulation (dashed line). The arrows show the corresponding sheath widths. Excitation frequency 25 MHz, for 3 W power in the plasma.

Figure 6: Sheath width dependence on excitation frequency at 3 W and 7 W power in the plasma. The sheath width is given by parabolic reconstruction of the sheath potential.

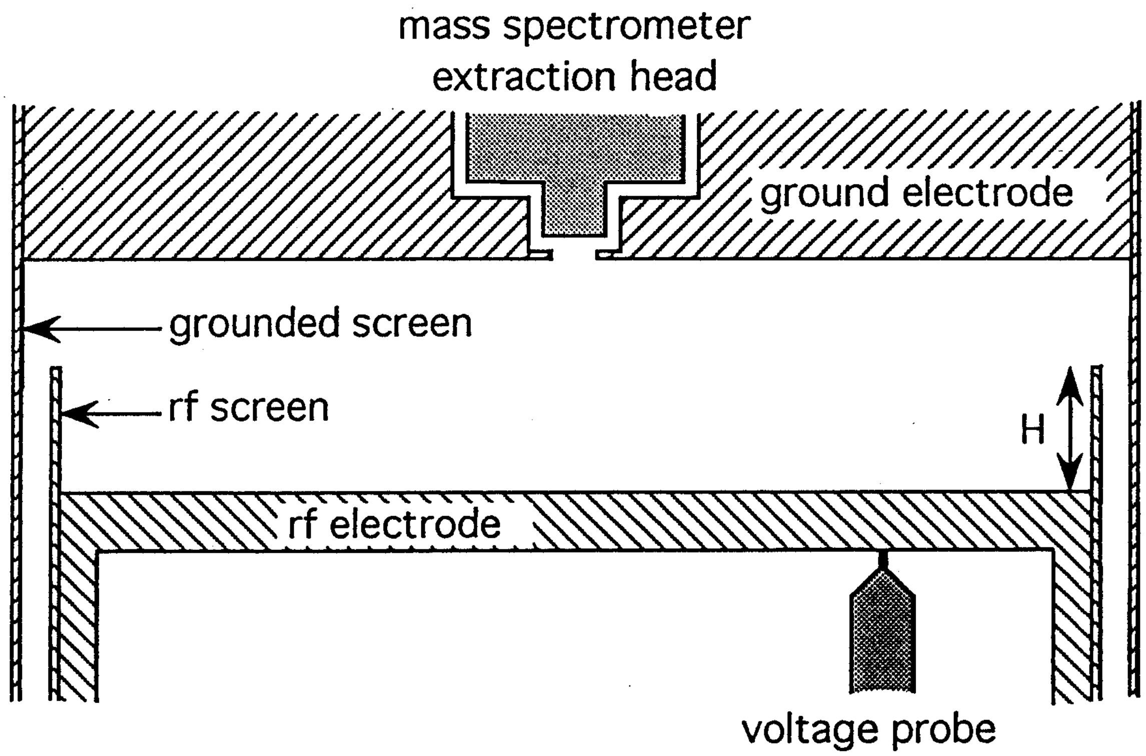
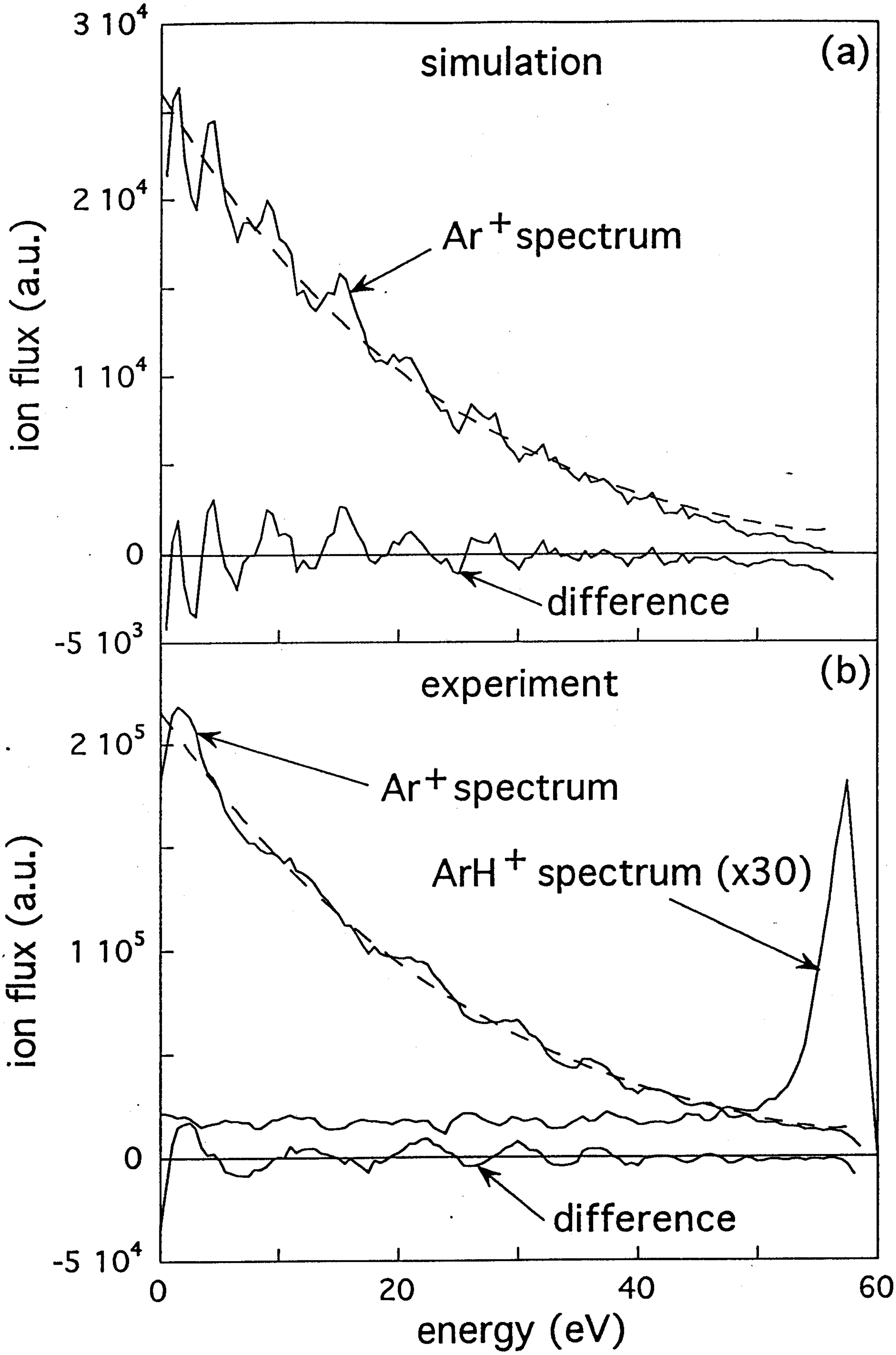

mass spectrometer
extraction head
ground electrode
grounded screen
rf screen
H
rf electrode
voltage probe

Fig. 1



3 10^4
2 10^4
1 10^4
0
-5 10^3
ion flux (a.u.)
simulation
(a)
Ar+ spectrum
difference
experiment
(b)
2 10^5
1 10^5
0
-5 10^4
ion flux (a.u.)
Ar+ spectrum
ArH+ spectrum (x30)
difference
0
20
40
60
energy (eV)

Fig. 2

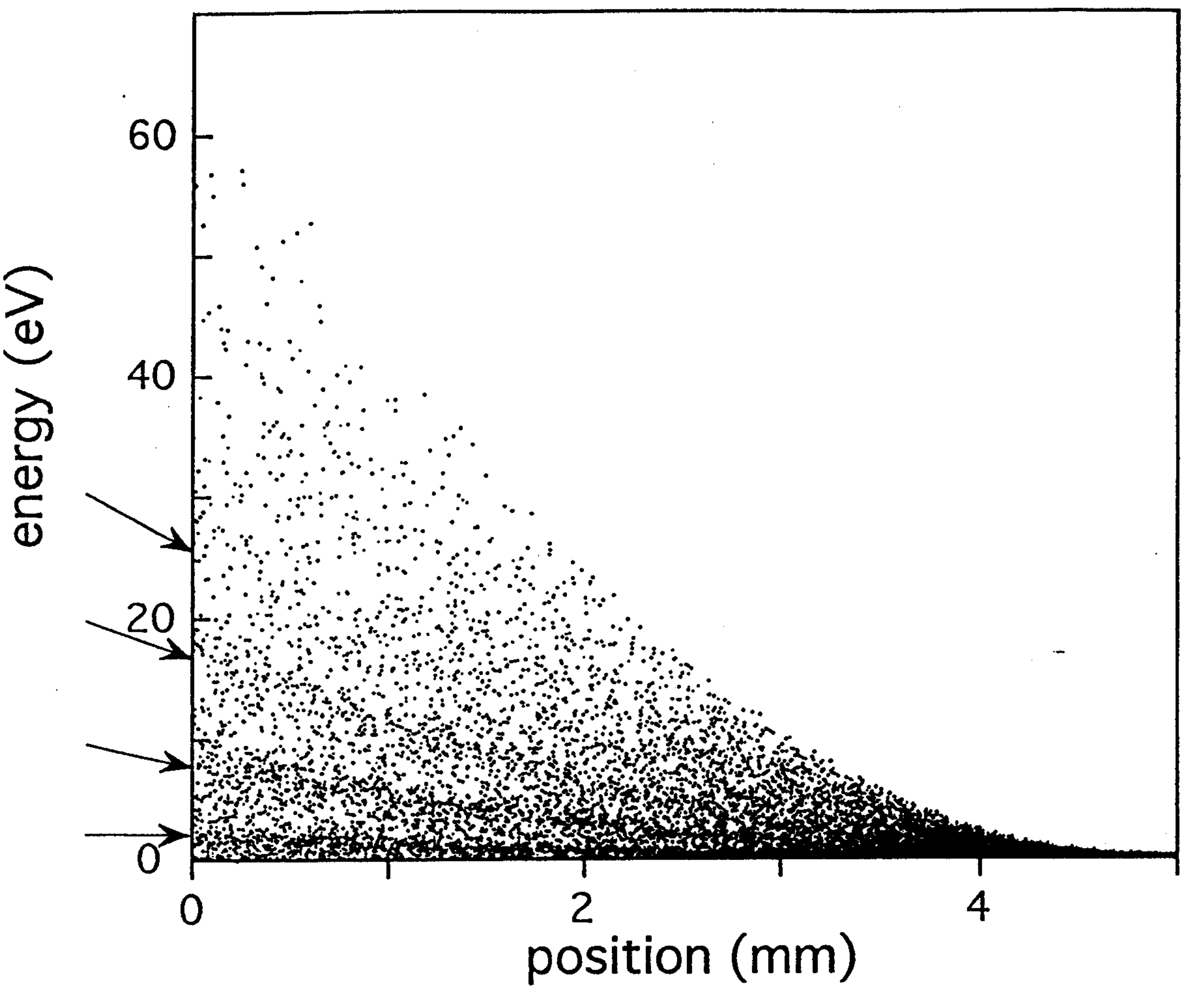


Fig. 3

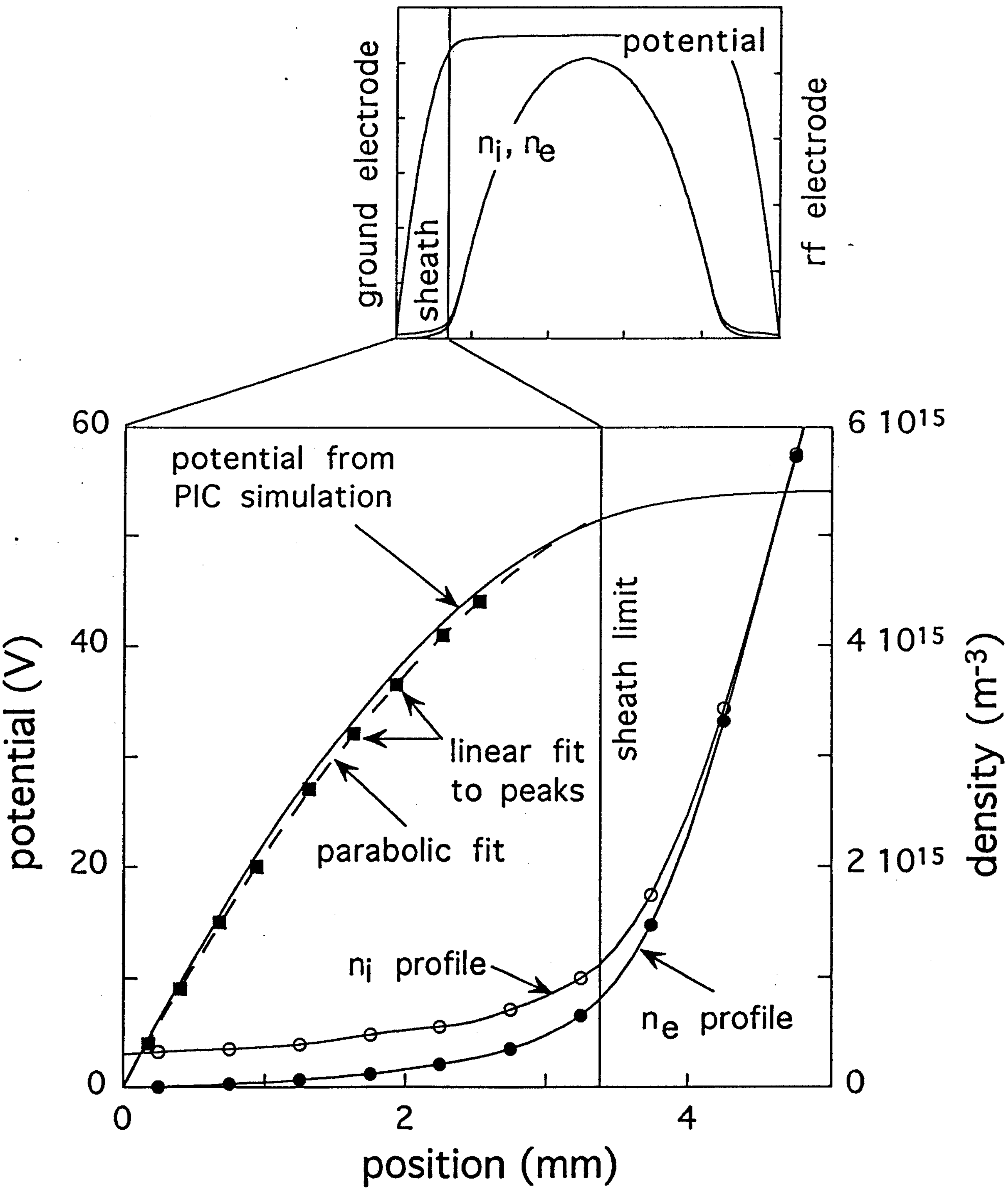
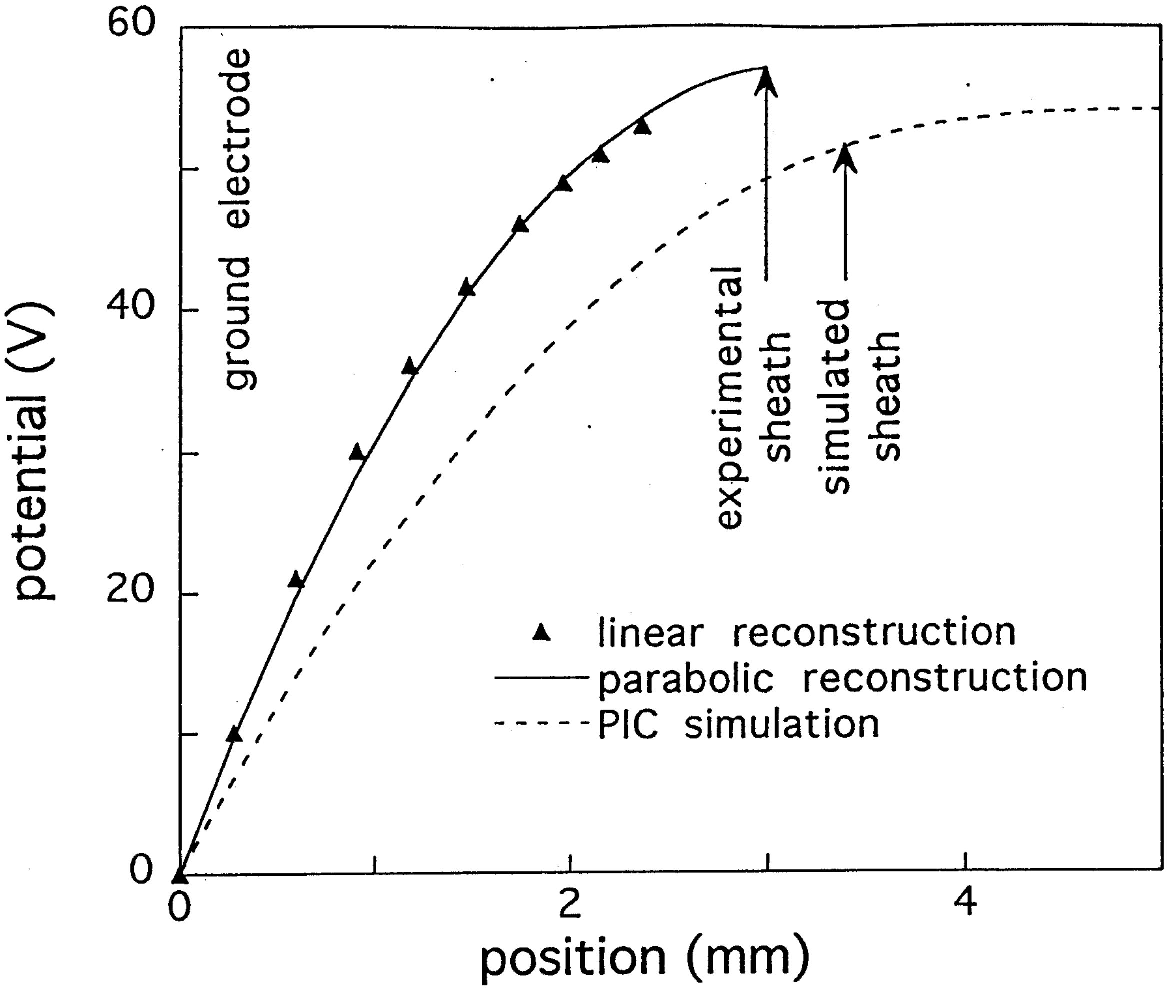
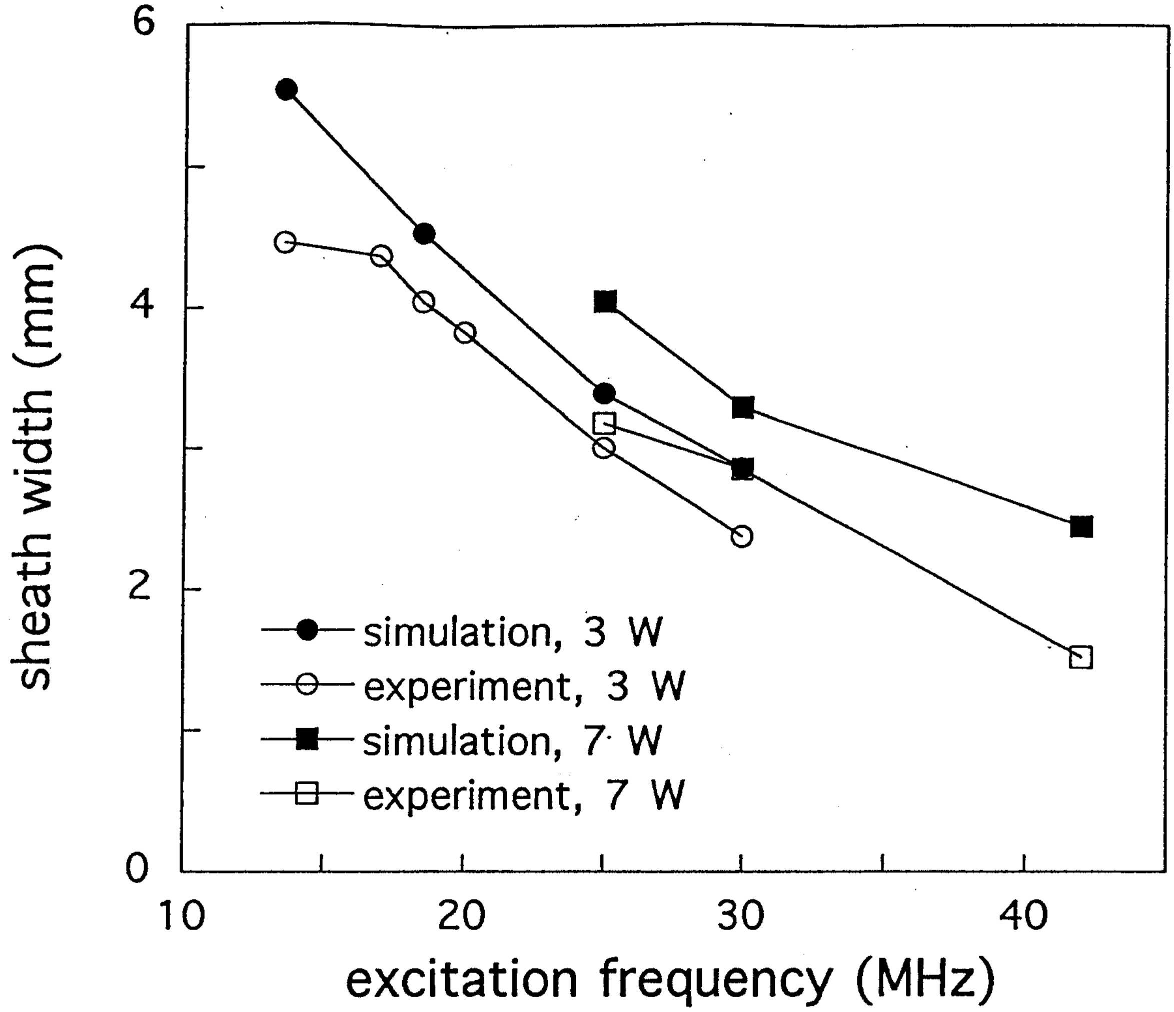

potential
ground electrode
sheath
n_i, n_e
rf electrode
60
40
20
0
0
2
4
potential from
PIC simulation
linear fit
to peaks
parabolic fit
sheath limit
n_i profile
n_e profile
6 10^15
4 10^15
2 10^15
potential (V)
density (m^-3)
position (mm)

Fig. 4



60
40
20
0
potential (V)
ground electrode
experimental sheath
simulated sheath
linear reconstruction
parabolic reconstruction
PIC simulation
0
2
4
position (mm)

Fig. 5



6
4
2
0
sheath width (mm)
10
20
30
40
excitation frequency (MHz)
simulation, 3 W
experiment, 3 W
simulation, 7 W
experiment, 7 W

Fig. 6