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Ion energy and angular distributions at the anode of RF etch reactors

P W May, D Field, D F Klemperer and Y P Song†
University of Bristol, School of Chemistry, Cantock's Close, Bristol BS8 1TS, UK

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Abstract. We present calculations of ion energy and angular distributions (IEDs and IADs) for ions striking the grounded electrode (anode) of RIE reactors. These distributions were calculated using a Monte Carlo simulation program incorporating a model for ion trajectories in the oscillating sheath region. We compare these IEDs and IADs to previously calculated distributions for the driven electrode (cathode). The effect upon the IEDs of varying the ratio of the area of the cathode:anode from 0.01 to 1.0 has been investigated. We also examine the effect upon IEDs of decreasing the frequency from 13.56 MHz to 100 kHz. IEDs for CF_3^+, CF_2^+ and CF^+ ions have been simulated and compared with experimentally observed distributions. Our calculated distributions closely resemble experimental IEDs, confirming that our simulations model anode processes as accurately as they model cathode processes.

1. Introduction

In order to understand the complex processes occurring at the surface of a semiconductor during plasma etching, it is necessary to have knowledge of the energies and angles at which ions from the plasma strike the substrate. High-energy ion bombardment of the wafer surface is fundamental to etch mechanisms, and it is the inherent directionality of the ions that is believed to be responsible for the mechanism of anisotropic etching.

We have recently developed expressions for some of the fundamental potentials occurring within RF systems [1]. Using these expressions we have written a Monte Carlo computer program that calculates the trajectories of ions as they travel through the oscillating sheath to strike the electrodes [2]. Our model only requires accurate knowledge of those plasma conditions which are readily obtained by simple measurements (e.g. RF voltage, DC bias and frequency). For low-pressure plasmas ($<$ 10 mTorr) the maximum sheath thickness can be obtained from visual observation of the extent of the dark space above the electrode [3]. At higher pressures, however, it is more accurate to calculate the sheath thickness from an expression derived by Morgan [4] and recently modified by May [2]. We also required approximate knowledge of the average ion and electron temperatures, but these can be readily estimated for most RF systems. Our model is not very sensitive to these two unknown parameters and consequently the errors introduced by a poor estimate will be small.

† Present address: University of Durham, School of Chemistry, Durham, UK.

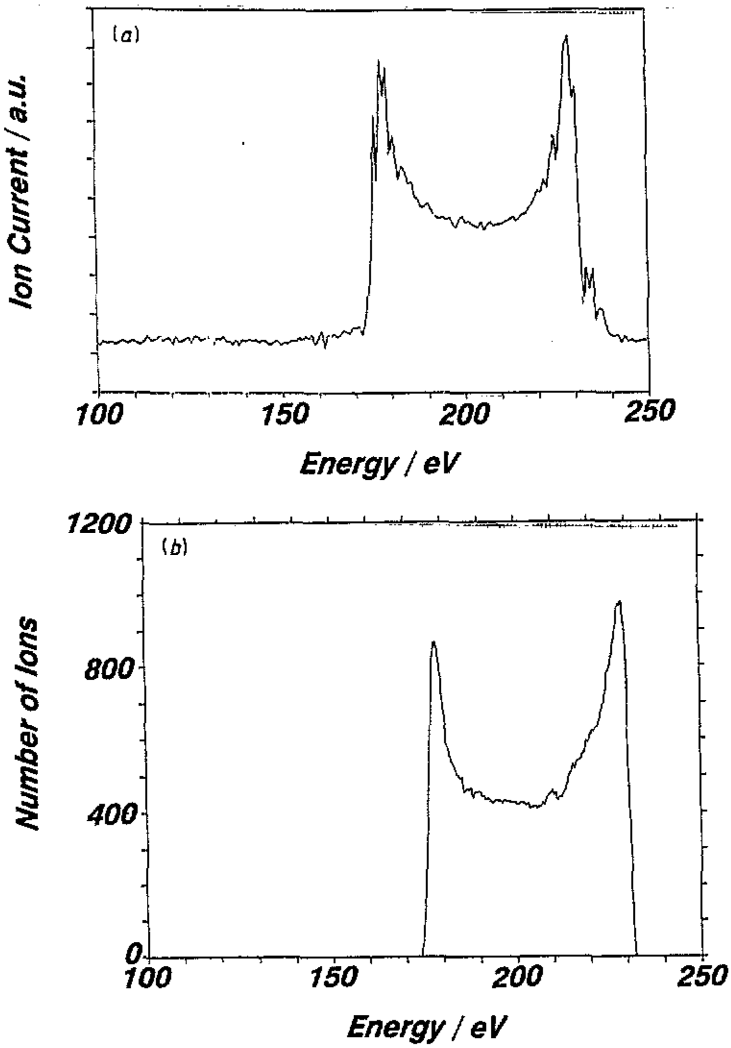


Figure 1. (*a*) Kuypers' [7] experimentally observed cathode IED for an Ar plasma at 2.4 mTorr: au = arbitrary units. (*b*) Simulation of the Ar^+ ion IED [5, 6] using the values for the plasma conditions given in the main text.

We have shown [5, 6] that our simulated IEDs for ions for striking the cathode in Ar, Ar/H_2, O_2 and CF_4 plasmas resemble those measured experimentally [7] extremely accurately. Using only the values for the plasma conditions quoted in [7] for the experimental etch process, we can reproduce both the precise shape of the observed IED, and also calculate the energies of the observed peaks to an accuracy of a few electron volts. Examples of cathode IEDs are given in figure 1 for an Ar plasma, where the close correspondence between our simulation and the observed distribution is apparent.

We have studied cathode IEDs and IADs extensively for both low- and high-pressure discharges [2] and we now extend our modelling to examine IEDs for Ar^+ ions striking the anode of RF systems.

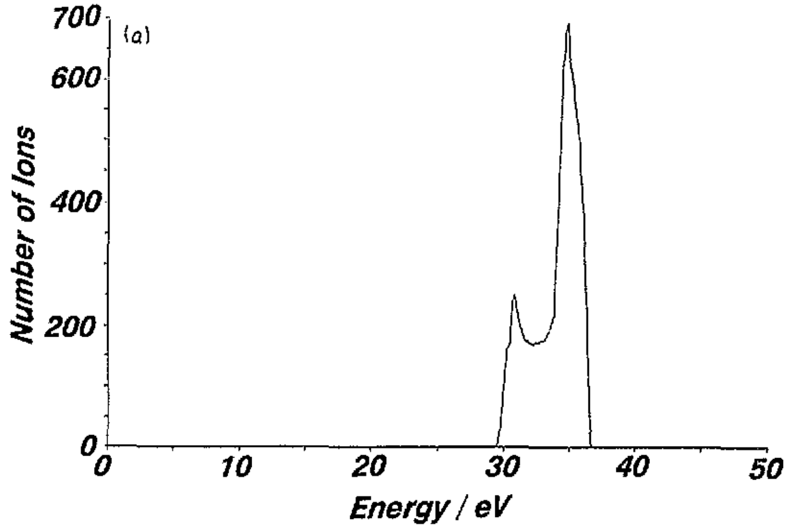
2. Results and discussion

We used the same plasma conditions that were previously employed to fit Kuypers' experimental cathode IED [7] (shown in figure 1) to calculate the IED at the anode. The conditions were: RF voltage $V_0 = 279$ V, maximum sheath thickness $l_{max} = 4.3$ mm, pressure = 2 mTorr, ratio of areas of cathode:anode $R = 0.4$, electron temperature $kT_e = 2$ eV, ion temperature $kT_i = 0.05$ eV and frequency = 13.56 MHz. To obtain an IED, we followed typically 10 000 ion trajectories. Each ion entered the sheath region with an initially randomly chosen RF phase and velocity. The initial velocity was chosen so as to be consistent with a Maxwell–Boltzmann distribution with the mean of 0.05 eV mentioned above. The low pressure of 2 mTorr is such that no collisions between the ions and neutral Ar atoms occur as the ions travel through the sheath region. Collisional effects such as scattering or charge exchange can have major effects upon IEDs [2].

The electrode area ratio of 0.4 is such that the cathode develops a significant DC bias ($V_{DC} = 174$ V for these plasma conditions), so that ions may be accelerated through a cathode sheath potential of several hundred volts. This is reflected in the high energies exhibited by the IEDs in figure 1. It is for this reason that semiconductor wafers are often placed upon the cathode (the so-called *RIE mode*) in order to utilize fully the resulting high-energy, directional ions.

In contrast the anode sheath potential is very small, being in general only a few tens of volts. As a result the sheath thickness is also much smaller than that seen on the cathode, in this case having a calculated maximum value of 1.54 mm. Therefore in general ions obtain little energy in crossing the anode sheath and strike the anode with only about 30 eV. This is illustrated in figure 2(*a*), which shows the calculated anode IED for the same plasma conditions as in figure 1. The characteristic double-peaked distribution is still evident, except that now the peak separation has been reduced from 55 to about 5 eV. Figure 2(*b*) shows the corresponding IAD. It is clear that, even though the anode sheath potential is small, ions still strike the anode at near-normal angles of incidence. In fact the spread of angles entirely reflects the initial velocity distribution of the ions, since those components parallel to the plane of the electrode will not be affected by the sheath potential. This result highlights why so-called *plasma-etch mode* reactors can still produce a certain degree of anisotropic etching, despite the lack of a DC bias contribution to the sheath potential. This type of etching, where wafers are placed on the anode, is still used in the semiconductor industry for features with large geometries (> 10 μm) and for processes such as resist ashing.

It is common for plasma-etch mode reactors to have electrodes of the same size. This results in no DC bias being developed on the driven electrode, but produces a large increase in the plasma potential. Figure 3 shows the effect upon anode IEDs of varying the electrode area ratio R from 0.01 to 1.0. For $R = 0.01$ the DC bias was calculated [1] to be 278.9 V, producing a total cathode sheath potential of 572.7 V. The corresponding anode sheath potential was therefore very small, having a maximum value of only 24.2 V. Hence the anode IED appears at low energies with a peak separation so small that the distribution appears as only a single peak. As R increases, the plasma potential increases and so the anode sheath potential and sheath thickness also increase. Hence the IEDs increase in energy and the peak separation becomes larger. For $R = 1.0$, i.e. equal area electrodes, the IED is identical on the anode and cathode. The average ion energy is now about 105 V with a peak separation of about 70 V.



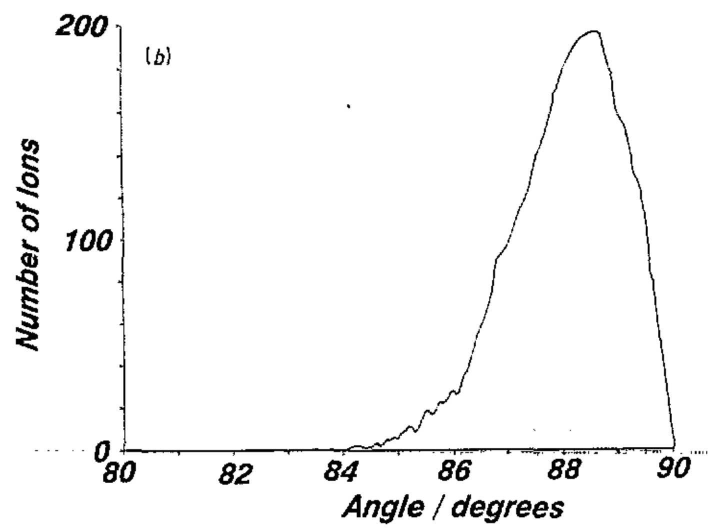


Figure 2. (*a*) Calculated IED for Ar^+ ions striking the anode for the same plasma conditions as figure 1 except with a value of l_{max} = 1.54 mm. (*b*) IAD for the same system. The angle of incidence is defined such that 0° is parallel to the plane of the electrode and 90° is perpendicular to it.

This shows that typical plasma-etch mode reactors can produce highly directional, energetic ion bombardment of the substrate. If such reactors are used for deposition rather than etching processes (e.g. PECVD), energetic ions might be a hindrance to film growth. A recommendation in this case, therefore, would be to decrease the size of the cathode.

Figure 4 shows an IED calculated at a frequency of 100 kHz. At this frequency the sheath boundary is moving so slowly with respect to the ions that it may be considered effectively stationary. Hence the IED directly reflects the form of the time variation of the anode sheath potential. The large peak at about 15 eV is caused by ions that encounter the sheath boundary when it has its minimum value. The form of the

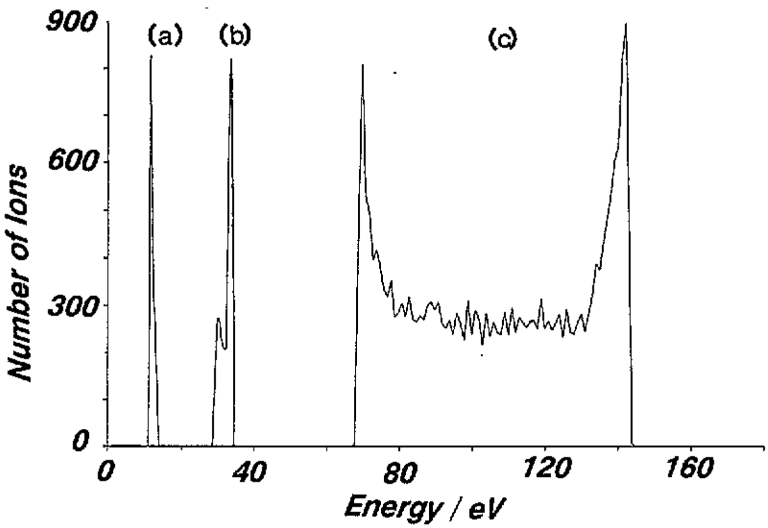


Figure 3. Calculated Ar^+ anode IEDs as a function of the electrode area ratio, R. All plasma conditions as for figure 2 except R = (a) 0.01, (b) 0.4 and (c) 1.0. The heights of the IEDs have been scaled so that they all fit on the same graph. In reality the area under each IED is equal.

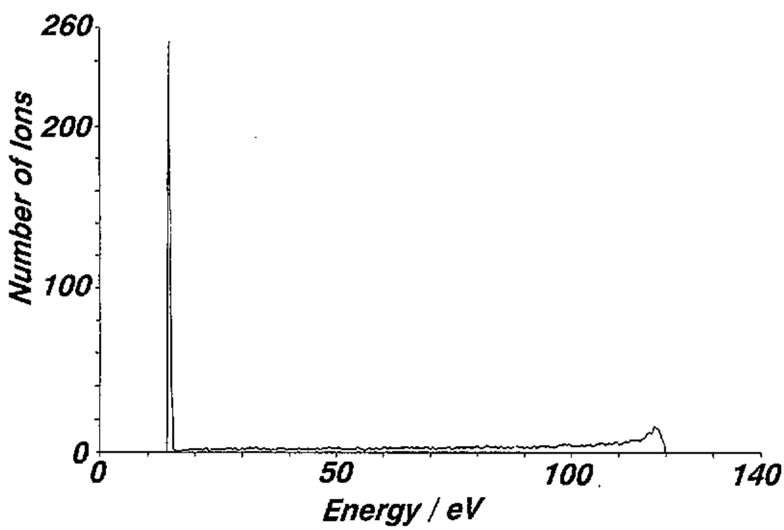


Figure 4. Ar^+ IED for the same plasma conditions as figure 2, except at a frequency of 100 kHz.

sheath potential is a rectified sinusoid [1], so that the sheath remains at this constant minimum value for about three-quarters of the RF cycle. Hence the peak at 15 eV is much the dominant feature of the low-frequency IED. There is another peak at about 117 eV which corresponds to those ions that encountered the sheath boundary when it had its maximum value. As the frequency increases the peak separation gradually decreases until at 13.56 MHz we obtain the IED of figure 2(a).

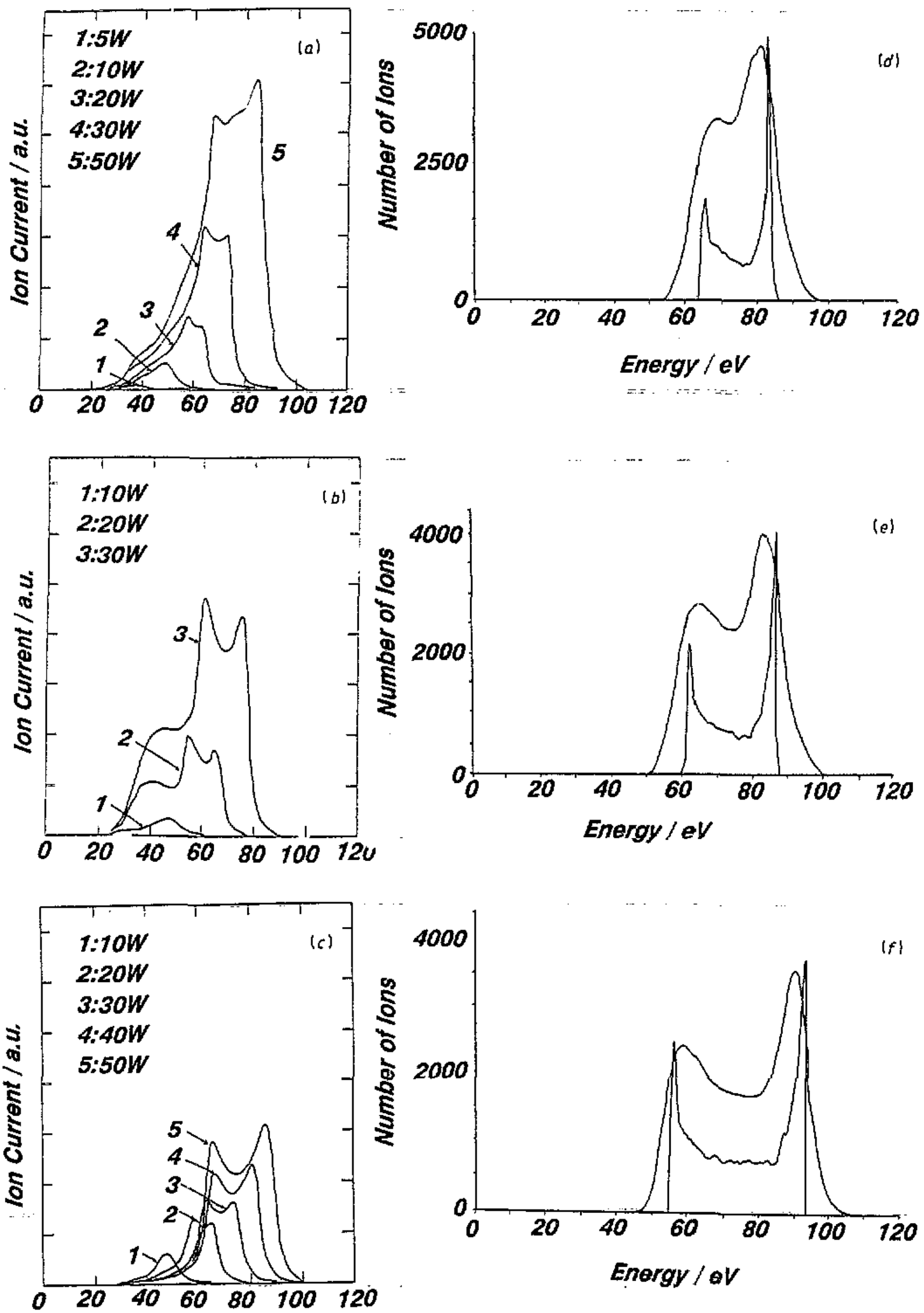


Figure 5. Experimental IEDs from a CF_4 plasma (after Bisschops [8]) using an equal area electrode reactor. Ionic species measured were (*a*) CF_3^+, (*b*) CF_2^+ and (*c*) CF^+. Our simulations of the 50 W IEDs are shown for (*d*) CF_3^+, (*e*) CF_2^+ and (*f*) CF^+. The two curves correspond to smoothing with an energy bin of 1 and 5 eV.

3. Comparison with experimental results

In order to test the accuracy of our anode IED simulations we have compared our calculations with IEDs observed in a real RF reactor. Bisschops [8] has measured IEDs on the anode of a plasma-etch reactor using a quadrupole mass spectrometer. Ions were sampled through a small hole in the anode and with this system he was able to resolve ions of different masses, so obtaining the IEDs for different ionic species. He used a CF_4 discharge, which gave rise to many types of ions, including CF_3^+, CF_2^+ and CF^+. Bisschops' experimental IEDs for these ions are given in figures 5(*a*), (*b*) and (*c*) for varying RF powers. These experiments were performed at a pressure of 13 Pa (about 100 mTorr), so collisional effects in the sheath will have affected the IEDs to a certain degree. This is most evident in figure 5(*c*) where a shoulder appears at the low-energy side of the main distribution. This shoulder is probably caused by charge exchange effects [2]. A small tail is also seen extending to low energies. This tail is due to the effect of various energy-loss processes in the sheath, such as scattering collisions between ions and neutrals [2].

Figures 5(*d*), (*e*) and (*f*) show our calculated IEDs for the 50 W plasmas. The plasma parameters used were Bisschops' quoted values for frequency = 13.56 MHz, $R = 1.0$, and $kT_e = 3$ eV, along with an estimated value kT_i of 0.05 eV. Unfortunately Bisschops does not quote values for V_0 or l_{max}, so these were used as fitting parameters. The IED for CF_3^+ was then simulated and the values of V_0 and l_{max} adjusted to obtain the correct energy and peak separation of the distribution. The other two distributions were then calculated using these fitted values to obtain the CF_2^+ and CF^+ IEDs without changing any of the parameters. The simulated IEDs are plotted with a resolution of 1 and 5 eV, the latter being chosen to simulate Bisschops's quoted experimental energy resolution.

It can be seen that the calculated IEDs resemble quite closely those seen experimentally. The general shape of the IEDs are very similar to those observed, with the exception that the small tail extending to lower energies has not been predicted since collision processes in the sheath were not included in the present model. Bisschops did not measure a 50 W CF^+ IED, so our simulation (figure 5(*f*)) serves as a prediction which clearly agrees with the experimental trend in figure 5(*c*).

This set of calculations serves to show that if all the required plasma parameters are not known, all that is needed to simulate accurately a complex gas IED are the values of the average energy and peak separation for *one* of the constituent ionic species, since this effectively calibrates the system. After fitting values of V_0 and l_{max} to this one IED, the IEDs for all the other ionic species can then immediately be calculated, although the relative contribution of each type of ion will still be unknown.

4. Conclusions

We have shown that by use of a Monte Carlo computer program we can accurately predict IEDs at the anode of RF systems. Ions typically strike the anode with much less energy than at the cathode, having in general energies of less than 50 eV. If the electrode areas are similar, however, ion energies on the anode can reach values of a few hundred electron volts, allowing anisotropic etching to occur.

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