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Self-consistent particle simulation of RF discharge in argon based on detailed collision data

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In order to obtain reliable computational data comparable with experimental data, self-consistent particle simulations of rf discharge in argon are performed by using the most accurate numerical procedure together with the most detailed collision data that are available now. In electron–atom collisions not only elastic and ionizing collisions but also 25 exciting collisions are taken into consideration one by one. In ion–atom collisions both elastic and charge-exchange collisions are considered by using the model whose validity is ascertained by measured data. Since no ambiguous approximations or assumptions are used, the obtained results can be regarded as standard data for rf discharge simulation. Copyright © 1996 Elsevier Science Ltd.

Key words: RF discharge, plasma, particle simulation, PIC method.

Introduction

Radio-frequency (RF) gas discharge is widely used in plasma processing technologies such as etching and sputtering.[1] Numerical simulation of RF discharge has been performed using the continuum model[2,3] for higher pressure and the particle model[4–8] for lower pressure. Our concern is in the latter case. We have chosen the particle-in-cell/Monte Carlo (PIC/MC) method[9] with some modifications.[10] The method can handle the nonlocal and nonequilibrium effects that dominate low-pressure glows without *ad hoc* assumptions.

The main purpose of the previous works[4,5,8] was to examine the qualitative structure of glow discharge in some model gas by using simplified collision cross sections. Surendra and Graves[6] took into consideration more realistic cross sections and scattering law. They treated helium because the light positive ion mass allows the PIC/MC simulation to converge to a solution more quickly. We consider the rf discharge in argon, which is much more important in applications. Trombley *et al.*[7] considered this problem by using the PIC/MC method. However, the electron- and ion-collision cross sections used in their simulation appear to be not so reliable, e.g. a large extrapolation to the high energy part may be done in electron-collision cross sections. Also, the validity of isotropic scattering used is not clear. The purpose of the present work is to obtain the most reliable results for argon discharge by excluding as many ambiguities in cross section data and simulation procedures as possible.

Simulation method

Overall procedure. The argon rf discharge in a parallel-disk reactor is simulated self-consistently. One electrode is powered by a RF voltage source at 13.56 MHz and the other is grounded. The computational domain is the inside of the cylinder with radius R and length D, where R is the radius of the electrodes and D is the distance between the electrodes. Although we here consider one-dimensional discharge, such a domain is used for a future extension to axisymmetrical discharge. Initially, a uniform plasma prevails in the whole domain. The weighting factor W is fixed at time zero. Each particle represents W particles in an actual discharge at any time. Time is advanced by Δt_e for electrons and by $\Delta t_i (= 30\Delta t_e)$ for ions. The equation of motion is solved by the use of the modified Verlet scheme. Electrons (e^-) and ions (Ar^+) incident on the cylindrical surface are specularly reflected. Electrons are absorbed and ions are neutralized on the electrodes. The secondary-electron emission coefficient γ was set to 0. The particles move in the three-dimensional space. Note that they are not the charged sheet in the one-dimensional PIC method. If a particle collides in a time step, its velocity is replaced by the post-collision velocity. The electric field E is calculated at the end of every time step Δt_e by use of the space charge distribution. The obtained field is used in solving the equation of motion for a new time step. In steady state, physical properties are sampled at a synchronous phase in lots of rf periods.

Collisions. As for e^-–Ar collisions, a set of detailed cross section data[11] in Figure 1 is used; 25 exciting collisions are separately taken into consideration in addition to elastic and ionizing collisions. The broken line with an arrow should be read by the upper scale. The total number of collisional events is 27. The probability of occurrence of the kth event in Δt_e is

$$P_k = N_A \sigma_k(\epsilon)\sqrt{2\epsilon/m}\Delta t_e,$$

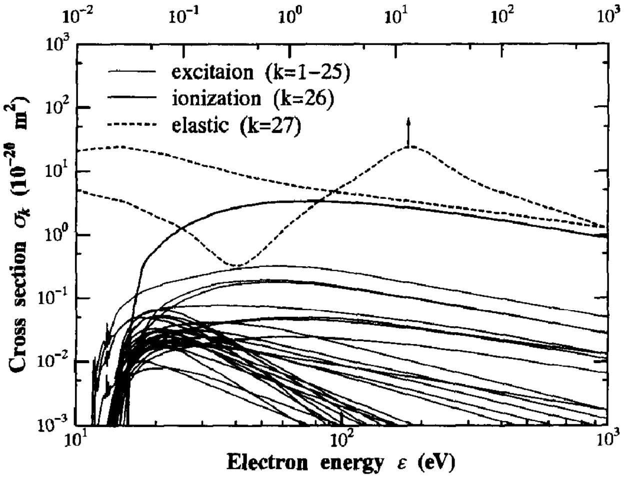

Figure 1. e$^-$–Ar collision cross sections.

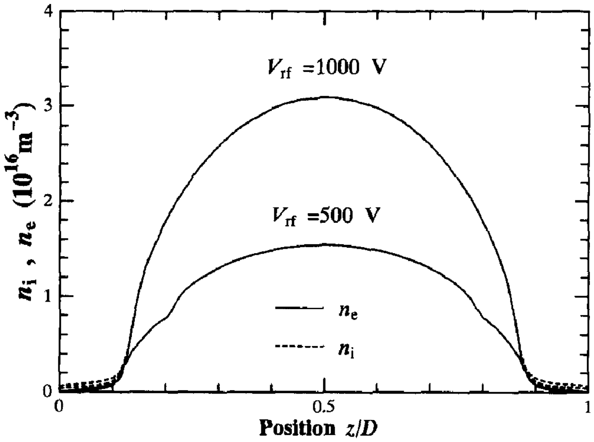

Figure 4. Densities of ions and electrons.

where N_A is the number density of Ar, σ_k the cross section of the kth event, ϵ the kinetic energy of e$^-$, and m the mass of e$^-$. Whether an electron collides or not in Δt_e and which event occurs can be determined by use of a single random number.[12] The post-collision velocity is determined based on a reliable model. Details are in Ref. 10. Elastic and charge-exchange collisions are considered in Ar^+–Ar collision. We use the collision model[13] which can reproduce all experimental data of drift velocity. The model holds good even for a very strong electric field considered here. The cut-off value of dimensionless impact parameter in the model is set to 9.

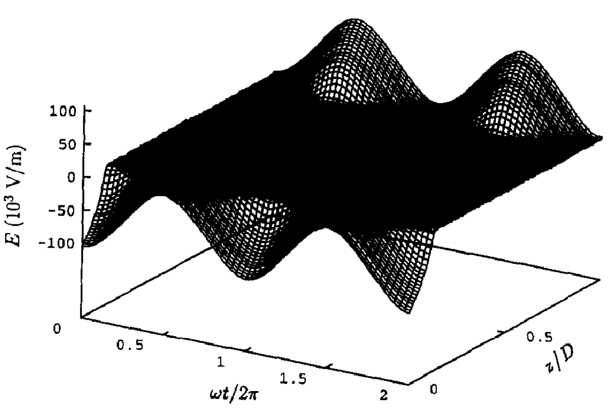

Figure 2. Spatio-temporal distribution of electric field.

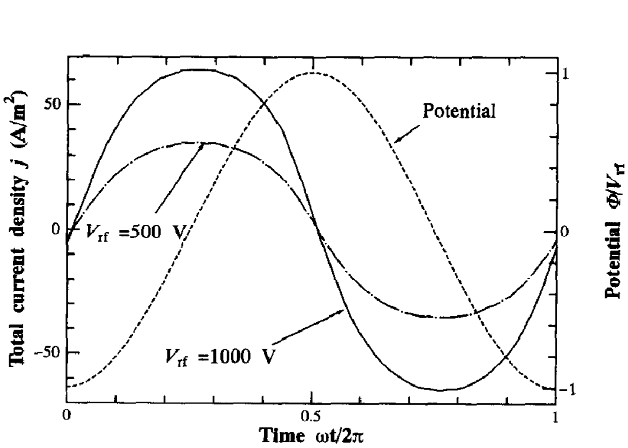

Figure 3. Total current density.

Results

Discharge conditions are as follows. The distance between the electrodes is 64 mm. The peak-to-peak RF voltage ($= 2V_{RF}$) is 200–2000 V. Argon pressure (p_A) is 42–74 mTorr. The time step Δt_e, at 42 mTorr is chosen to be 1/1920 of the RF cycle. Here we give the results for 42 mTorr unless stated otherwise. Other data are available from the authors. The potential at the powered electrode at $z = 0$ is set to $-V_{RF}\cos\omega t$, where $\omega = 2\pi f$ ($f = 13.56$ MHz) and t is the time. Figure 2 shows the spatio-temporal distribution of the electric field $E(z, t)$ for $V_{RF} = 500$ V. The thickness of the sheath oscillates as in the case of higher pressure.[3] The time-averaged potential V_p in the bulk plasma can be expressed as $V_p = 11.2 + 0.395V_{RF}$. The total current is the sum of conduction and displacement currents. The latter is dominant in the sheath and almost zero in the bulk, whereas the conduction current shows an exactly opposite behavior. Figure 3 shows the total current density j compared with the potential Φ at the powered electrode. The phase shift of j is 81°. It is the same for $V_{RF} = 500$ and 1000 V. The discharge is nearly capacitive. The electric field E at the powered electrode is always negative in a RF period. Because of the inertia of heavy ion, the ion current to this electrode is almost time-independent. Response of the electron to the electric field is very rapid. Since E is negative, electrons are repelled from the electrode. We found that the electrons can hit the electrode only when $|E|$ is very small. This period is only 20% of the RF cycle.

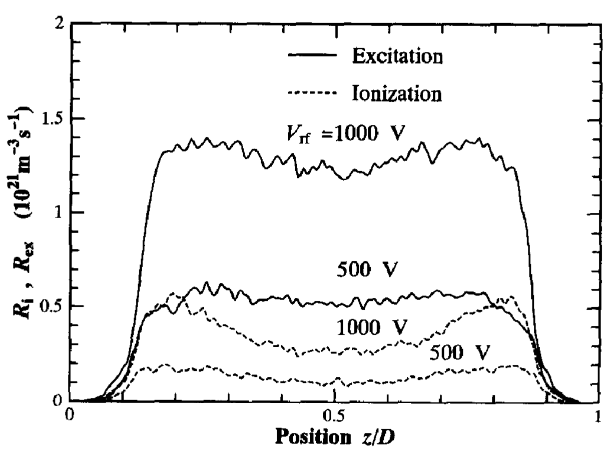

Figure 5. Rates of ionization and excitation.

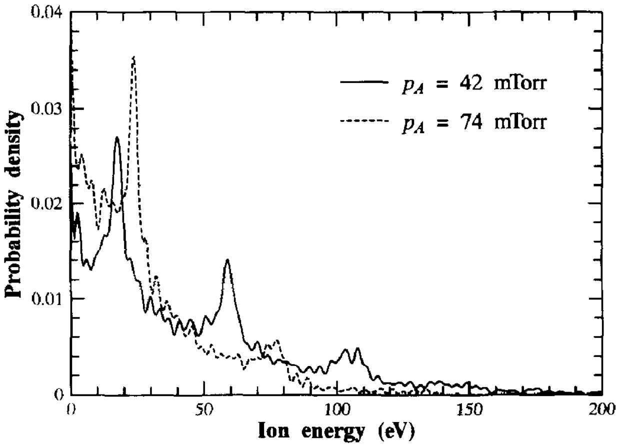

Figure 6. Energy distribution function of ion (V_{rf} = 500 V).

Figure 4 shows the time-averaged number densities of ion (n_i) and electron (n_e). If V_{RF} is doubled, the maximum density is also doubled. The profile is almost symmetrical with respect to the mid-plane. Figure 5 shows the ionization rate R_i and excitation rate R_{ex}. The latter is the sum of 25 excitation rates. Since electrons are accelerated in the sheaths of the two electrodes, R_i and R_{ex} take a maximum value near the sheath edges. The rates are rather high in the bulk. This is due to the forward scattering model used in our simulation. Figure 6 shows the time-averaged energy distribution function of ions incident on the grounded electrode for p_A = 42 and 74 mTorr and V_{rf} = 500 V. We see multiple spikes superimposed on a thermalized profile. Such spikes were also found in rf discharge in helium.[6] The number of spikes is equal to the number of charge-exchange collisions in the sheath. The locations of such collisions are supposed to be almost fixed.

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