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Brief Communication

Particle-In-Cell Monte-Carlo Simulation of Capacitive RF Discharges: Comparison with Experimental Data

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Particle-in-cell (PIC) simulations with Monte Carlo collision (MCC) are performed in argon capacitive rf discharges for the comparison with experimental data. The electron density and electron temperature along with the electron energy probability function are calculated for various gas pressures. It is shown that the sufficient number of simulation particles is one of the critical conditions for the reliability of PIC-MCC simulation. From the simulation with a large number of superparticles, a good agreement with experimental data measured by Godyak *et al.* [Phys. Rev. Lett. **65** (1990) 996] is obtained.

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KEYWORDS: particle-in-cell/Monte Carlo method, comparison with experiment, electron density, electron temperature, electron energy probability function

Capacitively coupled plasmas (CCPs) are one of the most common plasma sources for etching and deposition. To extend our knowledge of CCPs, numerous experimental measurements have been performed along with analytic and numerical modelings.[1–4] Godyak *et al.*[3] measured electron energy probability functions (EEPFs) in argon rf discharges using a Langmuir probe with an improved energy resolution. With increasing gas pressure, the transition of the EEPF from bi-Maxwellian to Druyvesteyn type was found along with the changes in the electron density and temperature. Although Langmuir probe measurement is the most popular diagnostic method, much attention should be paid for the accurate interpretation of measured data. A laser Thomson scattering (LTS) system[4,5] has been devised for the reliable measurement of EEPFs. Using a LTS system, ElSabbagh[5] measured EEPFs in a similar condition with Godyak's experiment. However, the transition was not observed in his experiment and the EEPFs were bi-Maxwellian over pressures from 50 to 500 mTorr. Because of the limitation and the possibility of misinterpretation in experimental measurements, the analytic and numerical modelings are commonly used to validate experimental data. The sufficient reliability of the simulation result is increasingly required. In this study, we perform the particle-in-cell (PIC) simulations with Monte Carlo collision (MCC) and compare our results with experimentally measured data.

The PIC-MCC code XPDP1[6,7] is utilized to simulate a one-dimensional parallel plate discharge. Simulation conditions are the same as Godyak's experimental conditions:[3] an argon discharge with the symmetric configuration of the gap length of 2 cm. The rf current of 2.65 mA cm^{-2} at 13.56 MHz was applied to the electrode. The electric potential at the boundary is found by applying the continuity of current.[6] For the stability and accuracy of the PIC-MCC simulation, the restrictions on some numerical parameters such as cell size Δx and timestep Δt need to be considered.[7,8] In our simulation, we used 400 cells and the timestep of 8×10^{-12} s. In addition, there is the statistical noise inversely proportional to the number of superparticles in PIC simulation. Sometimes the statistical noise leads to the significant numerical heating or cooling.[9,10] To reduce the short wavelength numerical noise, the digital smoothing method[11] for the charge density was applied in our simulations. At the steady state, the total number of superparticles for electrons (or ions) in the system was made to be approximately 1.5×10^5.

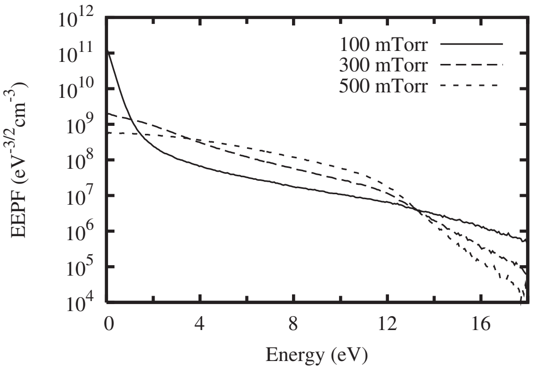

Fig. 1. The EEPFs obtained at the discharge center for different argon gas pressures.

Figure 1 shows the EEPFs at gas pressures of 100, 300, and 500 mTorr. The EEPF is defined as $f(\varepsilon) = F(\varepsilon)\varepsilon^{-1/2}$, where ε and $F(\varepsilon)$ are the electron energy and electron energy distribution function, respectively. As the gas pressure increases, the EEPF changes from bi-Maxwellian to Druyvesteyn type. This trend agrees well with that in Godyak's measurements[3] rather than that in LTS measurements.[5]

The electron density and electron temperature ($T_e = 2\langle\varepsilon\rangle/3$) calculated at the discharge center are also compared with those measured experimentally by Godyak *et al.* in Fig. 2 as a function of gas pressure. Vahedi *et al.*[12] compared their PIC-MCC simulation results with Godyak's experimental ones. At low pressures, they obtained smaller electron density and larger electron temperature in their simulation than those in the measurement by roughly a factor of two. The quarter of the total number of superparticles used in our simulation was used in their simulation for the same number of cells. In comparison to their simulation results, the electron density and electron temperature obtained in our simulation (Fig. 2) are in better agreement with those in Godyak's measurement under low pressure. To investigate the reason for better agreement, the simulation with one third of the total number of superparticles was performed at the gas pressure of 100 mTorr.

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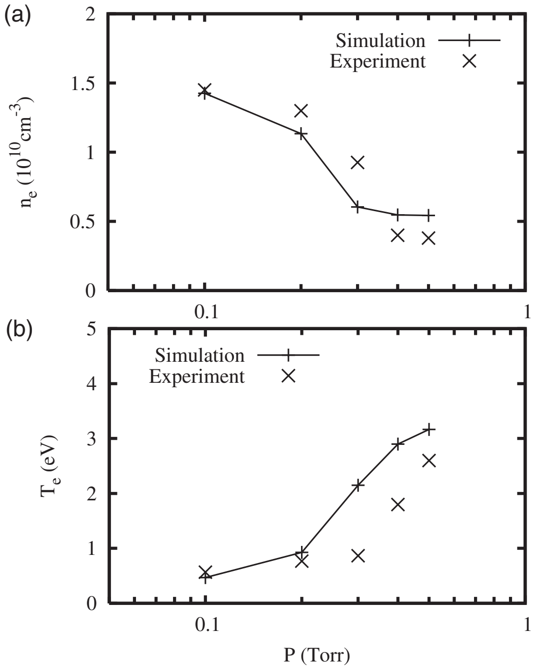

Fig. 2. (a) Electron densities and (b) electron temperatures at the discharge center as a function of gas pressure. The calculated values in our simulations are compared with the measured ones in Godyak's experiments.3)

Figures 3(a) and 3(b) show the spatial profiles of the electron density and electron temperature for two different numbers of superparticles, respectively. Figure 3(c) shows the EEPFs calculated at the discharge center. When the total number of superparticles is small, the electron density decreases and electron temperature increases by around a factor of 1.5. The EEPF also changes significantly especially in the range of low electron energy. A problem of statistical fluctuations of the electric field is severe especially at low gas pressures where most of plasma processings are performed.13) Since the electric field in the bulk is very small, the fluctuation of the electric field is significantly large and hence leads to the numerical heating of low-energy electron group. Thus, the sufficient number of superparticles is one of the critical conditions for obtaining the reliable PIC-MCC simulation result especially at low gas pressures. This is why our simulation results agrees well with the experimental data even under low pressure.

Acknowledgements

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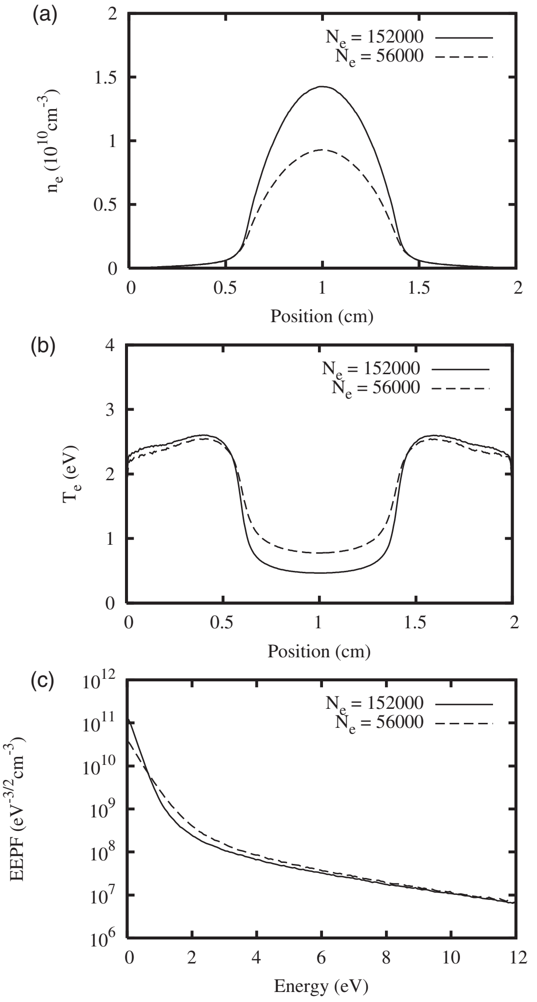

Fig. 3. The spatial profiles of (a) electron density and (b) electron temperature for different numbers of superparticles. (c) The EEPFs obtained at the discharge center for different numbers of superparticles. N_e represents the total number of superparticles for electrons in the system.

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