PIC/MCC Simulation of the Ionizing Characters in Electron Cyclotron Resonance Discharge

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Abstract A theoretical and computational model is presented to study the ionization of the argon electron cyclotron resonance (ECR) microwave discharge using a quasi-three-dimensional electromagnetic particle-incell plus Monte Carlo collision method. The interaction between the charged particles and microwave fields are described by the electromagnetic mode of particle-in-cell method. The collision processes are treated with Monte Carlo method. The simulation code is the original work. The results of the particle simulation for the ECR discharge of argon gas which include the microscopic features of charged particles and the electromagnetic characteristics of the ECR discharge plasma, and also the transient phenomena have been presented.

Key words electron cyclotron resonance discharge, particle-in-cell, Monte Carlo methods, ionization

1 Introduction

In recent year, electron cyclotron resonance (ECR) plasma has been extensively used in microelectronic fabrication^[1-3], such as chemical vapour deposition, etching, sputtering and so on. ECR ion sources (ECRIS) are attracting considerable attention for production of high-intensity multi-charged ion beams^[4-6] for accelerators, atomic physics experiments, and industrial applications. But the theoretical understandings for the ECR discharge phenomena, such as the ionizing characters of ECR discharge, are poorly understood.

Simulations performed with ECR plasma or ECRIS were mostly to predict physical quantities in their steady states up to the present. Although ECR plasma or ECRIS are normally thought of as stable output sources, the research on the process of discharge is meaningful^[7] for the more accurate simulation of the ECR plasma or ECRIS characters. Some fluid models^[8-10] were used to simulate the ECR

plasma production, and the time-dependent phenomena, such as: interchange instability, ion production, and electron heating are explored to research the time variations of hot-electron density, ion-trapping potential well, and core-electron temperature. But these fluid models couldn't study the microscopic features of charged particles, for example, the cyclotron resonance motion of electrons that is one of major phenomena in the ECR discharge. A one-dimensional electromagnetic particle-in-cell plus Monte Carlo collision method^[11] was presented to study the ECR discharge, showed the microscopic features of charged particles and the electromagnetic characteristics of the ECR discharge plasma, and also the transient phenomena. In this model, the electromagnetic wave is polarized circularly, and the trajectories are constructed from the integral of velocity.

In this work, we use a particle simulation method^[12] to study the ionization process of the argon ECR microwave discharge. The electromagnetic fields are calculated from the Maxwell equations.

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The motions of electrons and ions are determined by the equations of the relativistic motion and collision processes. The interaction between the charged particles and microwave fields are described by the quasi-three electromagnetic mode of particle-in-cell method. The collision processes are treated with Monte Carlo method. Elastic, excitational, and ionizing electron-neutral collisions and elastic, charge exchange ion-neutral collisions are included. The cross sections are the functions of particle's energy^[13-15].

The article is organized as follows: a brief review of the design features of the ECR reactor and the program flow chart of the PIC/MCC simulation are presented in Sec. 2, followed by discussions of the simulation results in Sec. 3. The conclusions are summarized in Sec. 4.

2 Modeling

The ECR reactor in this simulation is shown in Fig. 1.



Fig. 1. The ECR discharge reactor.



Fig. 2. Program flow chart.

The simulation code is the original work. The theoretical model is composed of three parts: the propagation of microwave, the weighting of current and the movement of charged particles. The program flow chart of the PIC/MCC simulation is shown in Fig. 2. It also illustrates the underlying method.

3 Simulation and discussion

The electron phase space plots are in Fig. 3 and Fig. 4. In Fig. 3(a), the electrons have very high perpendicular velocities near the center of the z axis where the external magnetic field is about 875 Gauss that makes $\omega \approx \omega_{c0}$. This means that the electron cyclotron resonance heating occurs there. The electrons absorb energy from microwave at the ECR region. Figs. 3(b—d) show that a lot of electrons have been created and the hot electrons localized near the ECR region at earlier times appear gradually over broad region. And the microwave is obviously damped here and can hardly propagate through this region, since its power is mostly absorbed at and near the ECR region, that is been presented in Figs. 4(a-d). But the fields here are again excitated by the current of new created charged particles with the process of ECR discharge.



Figures. 5(a-d) show the vz-vy phase space plots for electrons at four different times. We can see the electrons parallel velocities near the ECR region have not obviously increased that means the ECR heating only happens the perpendicular direction of the z axis. But these electrons undergo frequently collisions with neutrals and diffuse toward the boundaries of ECR reactor. As a result, the electron velocity distribution, that is strongly anisotropic in the direction of the z axis, gradually becomes isotropic.



Fig. 5. Vey-Vez.

The ion phase-space plots are given in Figs. 6(a-d)-8(a-d). The perpendicular velocity distribution of ions in Fig. 6(a) has the electric field form of the transverse wave, because the ions are modulated by the transverse electric field. Different from the electrons, the ions haven't the cyclotron resonance heating phenomena because of the mass of ion is much bigger than electron, the condition of $\omega \approx \omega_{c0}$ is not true. Figs. 6(b-d) show the ions created by the ionization electron-neutral collisions gradually diffuse over broad region.

Figure 7(a) illustrates that the most ions parallel velocities hardly increase result from the input microwave mode is TE mode and E_z is 0, except some ions parallel velocities are increased because of the ion-neutral elastic collisions that bring on the change of movement direction and the transform the momentum from perpendicular to parallel. Because of plentiful generation of ions and the frequently ion-neutral collisions, the ion velocity distribution, which was strongly anisotropic in the direction of the z axis, gradually becomes an isotropic distribution .This isotropization process can be seen in Figs. 7(b—d) and Figs. 8(a—d).



4 Conclusion

With a quasi-three PIC/MCC simulation code, we have studied the ionization characters of argon ECR discharge process. The propagation of microwave is researched, and the microscopic transient information about charged particles is obtained that including the distributions of electrons and ions in the Vy-z, Vz-z, Vy-Vz phase. The main conclusions can be drawn as follows:

(1) The ECR heating occurs at the region where $\omega \approx \omega_{c0}$, and the electrons absorb energy from microwave near the ECR region where the microwave power is coupled to them. The ECR heating is preferentially along the perpendicular direction.

(2) Many electrons and ions are created through the ionization collisions between electrons and neutrals at the ECR region at earlier times appear gradually over broad region.

(3)The distribution of charged particles vary gradually from anisotropic to isotropic by the frequently collisions with the process of ECR discharge.

The simulation results explain well the physical mechanism of the ECR microwave discharge which including the interaction between the charged particles and microwave, the propagation of the microwave, the transports of the charged particles.

Further studies of the dependence on the discharge parameters (the microwave mode, the microwave power, the neutral gas pressure, and the profile of the external magnetic field, etc.) will give us much more information on the ECR microwave discharge. These researches are in progress, and will be reported elsewhere.

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