KINETIC SIMULATION OF LOW PRESSURE RF DISCHARGE IN NONUNIFORM AXISYMMETRIC MAGNETIC FIELD

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An implicit 2D3V PIC/MCC code has been developed for the kinetic simulation of low pressure RF discharges. The code uses coupled particle-in-cell method (PIC) for calculation collisionless dynamic of the plasma particles and Monte-Carlo method (MCC) for taking in account the particle collisions. For the computation time reduction a number of physical and numerical methods of speeding up the code were introduced, such as the implicit schemes of the particles motion and fields computation, the electron sub-cycling and so on. The developed code is applied to the plasma dynamic investigation in capacitively coupled plasma RF discharge enhanced by the external magnetic field which is used in the neutral loop discharges (NLD).

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INTRODUCTION

RF discharges at low pressures, such as capacitively coupled plasmas (CCP), have played important roles as etching and deposition devices in semiconductor industry, as well as in some other applications, such as plasma lighting, displays and Hall thrusters. Computer simulation is an important tool, which helps to clarify its physical mechanisms. There are three commonly used simulation techniques, namely, the fluid, Particle-in-cell (PIC), and Boltzmann models in plasma physics research. PIC model solves the Newton and Maxwell equations directly. Kinetic, non-local and non-equilibrium effects can be included. PIC simulations of RF discharges are attractive because the fields and energy distributions can be obtained self-consistently from first principles. No assumptions need be made about the electric field or the bulk plasma velocity distributions, and the boundary conditions are realistic for both particles and fields. Collisions can be included in PIC simulations by coupling PIC methods with Monte-Carlo collisions (MCC). A detailed reference for PIC-MCC is provided in [1]. But PIC-MCC has a considerable disadvantage. It is computationally expensive compared to other numerical methods. Plasma simulations using fluid models run faster than PIC-MCC codes, but make assumptions about the velocity distributions of the electrons and ions and ignore kinetic effects such as stochastic electron heating. To keep the first-principle and self-consistent approach of PIC-MCC model while reducing execution time, the implicit 2D3V code was developed in axisymmetric geometry by introducing several numerical schemes. Then the code is applied to the plasma dynamic investigation in capacitively coupled plasma RF discharge enhanced by the external magnetic field which is used in the neutral loop discharges (NLD.

CODE DESCRIPTION

Numerous methods for speeding up PIC-MCC codes have been published in detail and widely applied, but usually one at a time (see, for example, [2]). In the developed code several speedup methods have been applied together to electrostatic simulations of RF discharges.

There are two kinds of algorithms, namely, direct implicit simulation and implicit movement method simulation. In the direct implicit method, the field equations are given by extrapolation of the particles equations of motion [3]. In the implicit movement method, the field equations are given by solving the lower fluid moment equations each cycle in conjunction with Poisson's equation for an implicit electric field and then by advancing the particle equation with this predicted electric field [4]. The code uses the direct implicit simulation method by Landon and Friedman [3]. The essence of this method is that the recursive filtering of the electric field damps out high frequency modes. If we apply the simple harmonic oscillator model to the implicit scheme, we obtain the following characteristic equation:

$$(2\xi-1)\left[(\xi-1)^2+\frac{\omega_{c\alpha}^2\Delta t^2}{4}(\xi+1)^2\right]-\omega_0^2\Delta t^2\xi^3=0\,, \quad (1)$$

where $\xi=\exp[-i\omega\Delta t]$, $\omega_{c\alpha}$ is the cyclotron frequency, ω_0 is a frequency of the external filed and Δt is a time step. With $(\omega_{c\alpha}\Delta t)^2<<1$ and $\omega_0\Delta t<<1$ the equation (1) gives the relative error in real and imaginary parts of the oscillation frequency: $|\mathrm{Re}(\delta\omega/\omega_1)|<1.05\omega_1^2\Delta t^2$, $|\mathrm{Im}(\delta\omega/\omega_1)|<0.75\omega_1^3\Delta t^3$, where $\omega_1=(\omega_0^2+\omega_{c\alpha}^2)^{\frac{1}{2}}$. For $\omega_0\Delta t>>1$ there is the root that corresponds to strongly damped oscillations:

$$\xi=\left[1+tg^2(\omega_{c\alpha}\Delta t/2)\right]^{\frac{1}{3}}(\omega_0\Delta t)^{-\frac{2}{3}}. \quad (2)$$

This implies that the high frequency oscillations are strongly damped while low frequency oscillations are weakly affected. Thus, the physics that is not accurately resolved by the use of large time steps is removed by the damping.

With the time steps used in order to satisfy stability and accuracy conditions for the electrons, the considerably more heavier ions make very short advance in one electron time step. Hence, the ions might be moved less frequently, every k^{th} electron time step, where k may be from 10 to 100, depending on the ion mass. To exploit the difference in inertia of ions and electrons the code uses the numerical technique that is called "sub-cycling" [6]. For each complete cycle of time integration, there is one cycle for the ions and several sub-cycles for the electrons. As the mass of ions makes them insensitive to high frequencies, one can use a larger time step for ions

than electrons, which quickly makes the cost of pushing ions very low. This algorithm use the fact that ions do not respond to the high frequency waves. This allows suppression of the high frequencies in the field seen by the ions and permits to push them with a time-step larger than that used for electrons. The electron density is defined at integer time steps simultaneously with the ions, and at fractional time steps. Namely, the ion density is known at time $t_n = n\Delta t$, while the electron density is known at time $t_{n/N} = (n/N)\Delta t = n\Delta t_e$. Electrons are pushed from time $n\Delta t_i - M\Delta te$ to time $n\Delta t_i + M\Delta te$, where $M = (N-1)/2$, assuming ion positions as defined at time $n\Delta t$. The electric field seen by the ions is then computed as a function of the electric field calculated from the intermediate positions of electrons. Ions are then advanced one time step and the cycle is repeated.

The PIC-MCC simulations usually continues while the density profiles evolve to their equilibrium states. With initial spatially uniform ion and electron density profiles it takes the long computation time. The time to reach equilibrium is improved by starting off with non-uniform initial density profiles that are close to their final equilibrium values. These profiles are deduced from previous runs or may be estimates from physical considerations.

One method of obtaining a better initial starting point for a simulation is the use of "light ions" [7]. The light ion speedup method is done in two steps. First, the real ion masses are replaced with the light ion masses and simulation runs until it comes to a "light ion" equilibrium. Reducing the mass of the ions increases their speed, which enables them to reach an equilibrium state in a smaller number of RF cycles, and hence less computer time. Then the real masses are restored, and run until equilibrium again. The overall running time is found to be less than that running with the real ion mass throughout, since the light ions reach equilibrium faster than real ions.

CCP-NLD DISCHARGE SIMULATION

As an application of the code the simulation of the low pressure RF discharge enhanced by the nonuniform magnetic field was carried out. The magnetic field topology is like in neutral loop discharges (NLD). In NLD inductive or capacitive plasma coupling may be used. The simulation of NLD with inductive coupled plasma was performed earlier in [8]. In this work the case of the capacitively coupled neutral loop discharge is considered (CCP-NLD). The NLD magnetic field configuration can be created by three coils that are placed coaxially around an axisymmetric discharge chamber. The currents of the first and last coils have the same direction, and the current of the middle coil has the opposite direction. The resulting magnetic field is axisymmetric with X-point. At X-point the magnetic field vanishes. The region near X-point, which is usually defined by the inequality $|B| < B_{ECR}$, forms toroid -like structure that is the neutral loop itself. Here $B_{ECR} = (m_e c/e)\cdot\omega_0$ is a magnetic field strength corresponding to the electron cyclotron frequency, which is equal to the RF frequency ω_0. For the RF frequency 13.56 MHz $B_{ECR} \approx 4.8$ G. Such magnetic coils configuration allows to change the position and the diameter of the NL contour by varying the currents in the coils. As a result the diameter of the plasma ring with maximum plasma density changes.

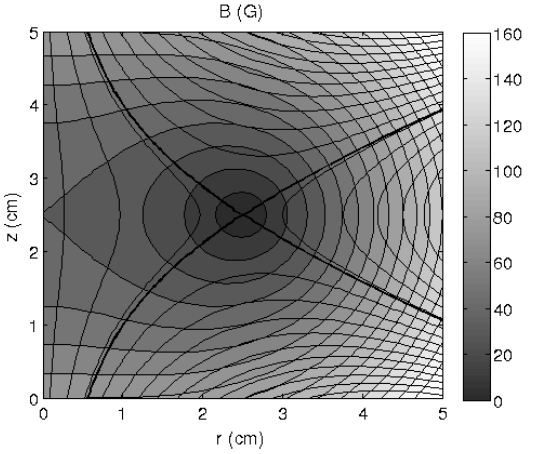

Fig. 1. Configuration of the magnetic field

A configuration of the external magnetic field near NL is shown in Fig. 1 in *r-z* plane. In this figure the magnetic field contour lines, the calculated profile of the magnetic field strength lines, X-point and separatrix are depicted. The radius and the axial position of NL are equal to 2.5 cm. The point where $B = B_{ECR}$ lies on the distance 0.6 mm from X-point.

The problem is solved in cylindrical geometry. The dimensions of the computational domain are as follows : the radius of the discharge chamber $R = 5$ cm, the axial extent $L_z = 5$ cm. The usual number of mesh points 64×64. Consequently the cell size is $\Delta r = \Delta z = 0.078$ cm. The operation gas is argon. The pressure values varies from 5 to 50 mTorr. Initial plasma profile is parabolic. The collisions between the electrons and the neutral background, including elastic scattering, excitation and ionization, are treated by the Monte Carlo method. The typical time step $\Delta t = 10^{-11}$ s. It is less than the fastest time scale in the discharge, which is defined either by the inverse electron plasma frequency, the inverse collision frequency, or the "grid travel time" $\Delta x/\overline{\upsilon}$, where $\overline{\upsilon}$ is the typical electron velocity. The electric field is calculated self-consistently by the PIC algorithm. The boundary conditions are determined by treating the bottom and top of the simulation domain as powered and grounded electrodes, respectively, while the mantle is a dielectric. At the powered electrode the RF voltage $V_{RF} = 50$ V is applied with the frequency 13.56 MHz. More than $5\cdot10^5$ super-particles are used in each simulation run to represent the plasma. This is large enough to avoid problems with artificial self-heating and other numerical noise errors. Every simulation runs for several thousand RF cycles to reach steady-state operation.

The simulation results show the strong influence of the magnetic field. In Fig. 2 the spatial profiles of electron energy distribution are depicted. In Fig. 2,a the electron energy distribution with presence of the

magnetic field is shown. For comparison Fig. 2,b shows the electron energy distribution for the case, when the external magnetic field is turned off.

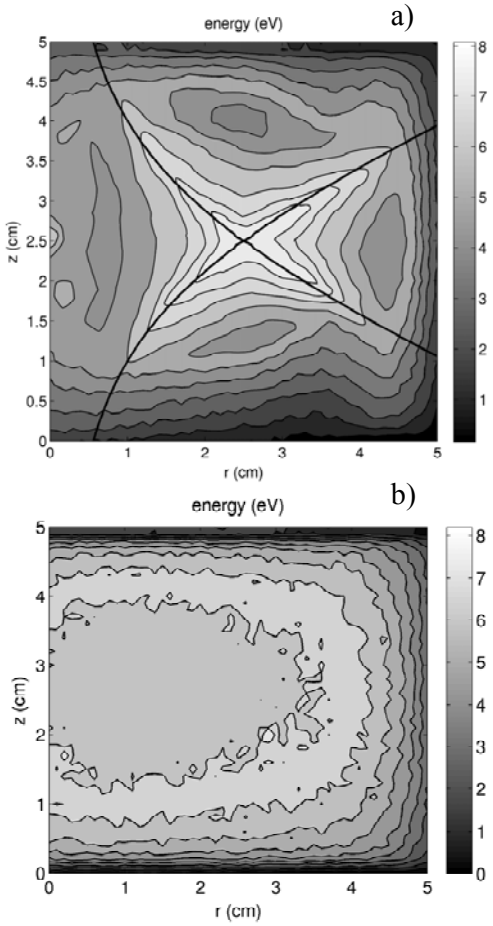

Fig. 2. Electron energy distribution with (a) and without (b) magnetic field (p = 5 mTorr)

Fig. 2,a shows that with the magnetic field turned on the maximum of electron energy is located at the neutral loop with a small shift from X-point outward. The electron energy is high also in adjacent regions which are linked with neutral loop by magnetic field strength lines. High electron energy in these regions is due to presence of the additional to collisional heating mechanism. Collisional heating becomes inefficient at pressures below 10 mTorr. However, in the magnetic field configuration with NL an alternative collisionless heating mechanism exists. Motion of the electrons far from the NL is regular. But in the region close to NL, where the magnetic field is low and inhomogeneous, the adiabatic invariance of the magnetic moment is destroyed, and the degree of freedom increases enough to generate chaotic motion of electrons.

In the process of electrons energy losing through inelastic collisions a sink of the energy in a high-energy region of the velocity space appears. A steady state is achieved when the same number of electrons are supplied from a low-energy region, and then they are moved towards the sink in the velocity space by the cascade process driven by the mixing effect. The chaos accelerates the cascade process, and enhances the energy dissipation into the sink. The energy dissipation is determined by the speed of the cascade, which is defined by the Lyapunov exponent, and the energy removal rate in the sink region [9].

On the other hand the electron energy is lower in zones, where electrons are magnetized. Here the electrons are confined by the magnetic traps and heated due to Ohmic dissipation, diffusion and heat transfer across the magnetic field which transport electrons and energy from the regions with higher magnetic filed to the lower ones. However, these processes are not effective in the low pressure discharges.

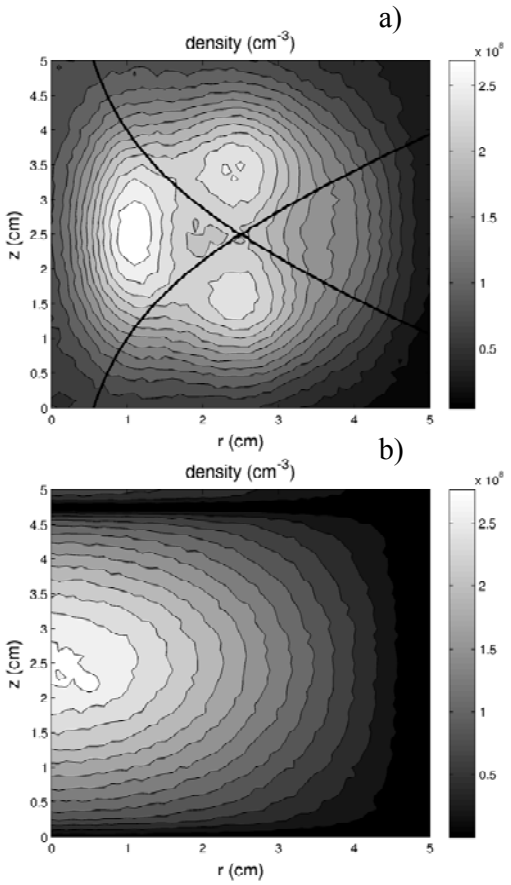

Fig. 3. Electron density distribution with (a) and without (b) magnetic field (p = 5 mTorr)

The computer simulation results show that the electron density profile has complex enough structure. In figure 3a the electron density profile is depicted for the turned on magnetic field, and Fig. 3,b shows the electron density without magnetic field. Fig. 3,a argues that the electron density near NL is inhomogeneous both in radial and axial directions. The density maximum is not located at the X-point but is shifted inwards in radial direction, and additional local maxima appear above and below the NL. This results qualitatively agree with several experimental studies, where such behavior of the electron density is explained by electron confinement in the local magnetic traps. Indeed, there are several magnetic traps in NLD as it can be seen from Fig. 1. Near these traps boundary of the high density region coincides with the magnetic surfaces.

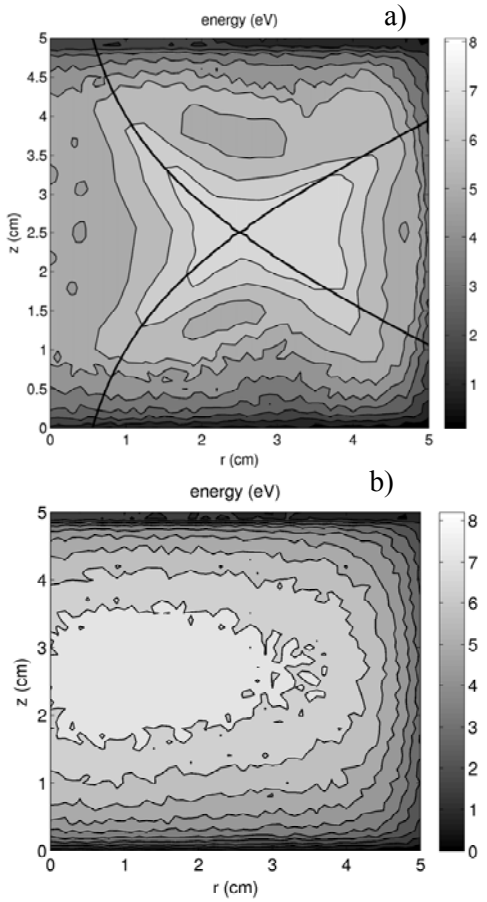

Fig. 4. Electron energy distribution with (a) and without (b) magnetic field (p = 50 mTorr)

At higher pressure, the plasma becomes more collisional. This increases the transport across the magnetic field lines and collision heating becomes more efficient. Therefore the spatial structures in the electron energy and the electron density become less expressed.

This is clearly seen in Fig. 4, where the electron energy distribution for more high pressure (50 mTorr) is presented.

CONCLUSIONS

The computer simulation results have shown that the stochastic heating mechanism exists in the NLD discharge and it is more effective at lower pressure.

REFERENCES

1. V. Vahedi and M. Surendra. Monte-Carlo Collision Model for Particle-in-Cell method: Application to Argon and Oxygen Discharges // *Comp. Phys. Comm*. 1995, v. 87, p. 179-198.

2. V. Vahedi, G. DiPeso, C.K. Birdsall, M.A. Lieberman, and T. D. Rognlien. Capacitive RF Discharges Modelled by Particle-in-Cell Monte Carlo Simulation. I: Anaylsis of Numerical Techniques //*Plasma Sources Sci. Technol.* 1993, v. 2, p. 261-272.

3. A.B. Langdon, B.I. Cohen and A. Friedman. Implicit Time Integration for Plasma Simulation //*J. Comput. Phys*. 1982, v. 46, p. 15-38.

4. R.J. Mason. Implicit Moment Particle Simulation of Plasmas //*J. Comput. Phys*., 1981, v. 41, p. 233.

5. C.K. Birdsall and A.B. Langdon. *Plasma Physics via Computer Simulation.* McGraw-Hill, 1985.

6. J.C. Adam and A. Gourdin Serveniere. Electron Sub-Cycling in Particle Simulation of Plasma. // *J. Comput. Phys.* 1982, v. 47, p. 229-244.

7. E. Kawamura, C.K. Birdsall and V. Vahedi. Physical and numerical methods of speeding up particle codes and paralleling as applied to RF discharges // *Plasma Sources Sci. Technol*. 2000, v. 9, №.3, p. 413-428.

8. A.V. Arsenin, V.G. Leiman, V.P. Tarakanov. Self-consistent simulation and analysis of the electron heating process in a neutral loop discharge // *13th International Congress on Plasma Physics.* Kiev, May 22-26, 2006, D018p.

9. Z. Yoshida et al. Anomalous Resistance Induced by Chaos of Electron Motion and its Application to Plasma Production. // *Phys. Rev. Lett.* 1998, v. 81, № 12, p. 2458-2461.

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КИНЕТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ВЧ-РАЗРЯДА НИЗКОГО ДАВЛЕНИЯ ВНЕОДНОРОДНОМ АКСИАЛЬНО-СИММЕТРИЧНОМ МАГНИТНОМ ПОЛЕ

В.В. Ольшанский

Для кинетического моделирования ВЧ-разрядов низкого давления разработан неявный 2D3V PIC/MCC код. Код использует метод «частица в ячейке» (PIC) для расчета бесстолкновительной динамики частиц плазмы и метод «Монте-Карло» (MCC) для учета парных столкновений частиц. Для сокращения компьютерного времени в коде применяются различные численные и физические методы ускорения расчета, такие как неявный метод расчета движения частиц и полей, электронные подциклы и другие методы. Разработанный код применяется для исследования динамики плазмы в ёмкостном плазменном ВЧ-разряде, усиленном внешним магнитным полем, используемом в разрядах с нейтральным контуром (NLD).

КІНЕТИЧНЕ МОДЕЛЮВАННЯ ВЧ-РОЗРЯДУ НИЗЬКОГО ТИСКУ В НЕОДНОРІДНОМУ АКСІАЛЬНО-СИМЕТРИЧНОМУ МАГНІТНОМУ ПОЛІ

В.В. Ольшанський

Для кінетичного моделювання ВЧ-розрядів низького тиску розроблено неявний 2D3V PIC/MCC код. Код використовує метод «частинка в клітинці» (PIC) для розрахунку динаміки частинок плазми без зіткнень і метод «Монте-Карло» (MCC) для врахування парних зіткнень частинок. Для скорочення комп'ютерного часу в коді застосовано різні числові та фізичні методи прискорення розрахунку, такі як неявний метод обчислення руху частинок і полів, електронні підцикли та інші методи. Розроблений код застосовується для дослідження динаміки плазми в ємнісному плазмовому ВЧ-розряді, підсиленому зовнішнім магнітним полем, що використовується в розрядах з нейтральним контуром (NLD).