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A PARTICLE-IN-CELL/MONTE-CARLO-COLLISION CODE FOR THE SIMULATION OF A 2.45 GHz LITHIUM ECR ION SOURCE*

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Abstract

A 2.45 GHz hybrid $^7Li^{3+}$ ion source has been designed at Peking University (PKU). In order to better understand the physical processes inside the hybrid lithium ion source, a Particle-in-Cell/Monte-Carlo-Collision (PIC/MCC) code is developed recently. In this model, the propagation of the 2.45 GHz microwave is processed using Finite-Difference Time-Domain (FDTD) method, and PIC and MCC method are used to handle the interaction of charged particles with electromagnetic field and collision process between particles, respectively. It can be used to simulate the motion of particles in single spatial dimension and three velocity dimensions, abbreviated as 1D3V. The validity of the PIC method has been confirmed by the simulation of two stream instability in this work. The preliminary simulation results show that the 2.45 GHz microwave energy can be absorbed effectively by electrons in the presence of an external magnetic field of 875 G. And the mirror magnetic field can increase the transverse velocities of electrons.

INTRODUCTION

To fulfil the requirement of the Compact Intense Fast NEutron Facility (CIFNEF) which is proposed by Peking University (PKU) and China Institute of Atomic Energy (CIAE), a 2.45 GHz hybrid ion source for the production of $^7Li^{3+}$ is designed [1]. Its schematic view is plotted in Fig. 1.

This hybrid $^7Li^{3+}$ ion source is composed of a hot surface ionizer and a 2.45 GHz microwave ion source. To get lithium vapour, an oven and a heater are used. In order to avoid the condensation of the lithium vapour, the transport pipeline and the liner are all adiabatic. The red boundary in Fig. 1 will be hot surface. Like other ECR ion source developed at PKU, a three-layer Al_2O_3 window plus a BN disc will be used to introduce the 2.45 GHz microwave into the plasma chamber. A minimum-B magnetic configuration generated by permanent magnets will be used to confine the plasma.

Electron Cyclotron Resonance (ECR) ion sources based on the minimum-B trap are efficient for the production of high charge state ions [2]. One of numerical models which paid more attention on the microwave in the ECR plasma was presented by Muta et al [3].

In Muta's model, a three-dimensional simulation of microwave propagation in an ECR plasma using finite-difference time-domain (FDTD) method has been presented. And the propagation characteristics of the microwave in an inhomogeneous plasma filled in a cylindrical chamber was investigated. In this work, ECR plasma was treated as an anisotropic, dispersive medium. Edgell et al developed a 1D spatially computer model for both electrons and multiple ion species in an ECR plasma [4].

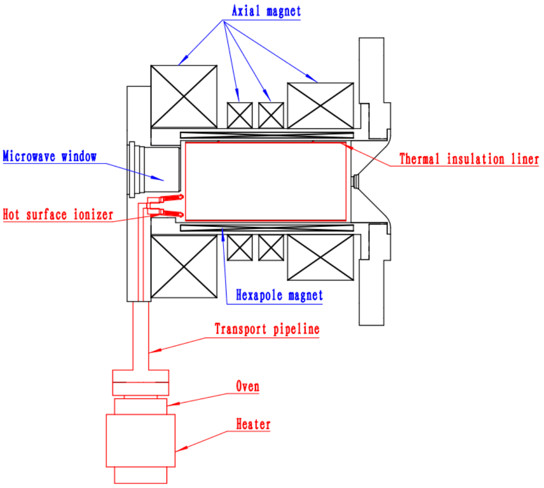

Figure 1: The schematic view of the structure of the $^7Li^{3+}$ ion source.

In that model, ECR heating was treated as a quasi-linear RF-diffusion term including relativistic detuning and RF pitch-angle scattering. Electrostatic models are also used in the simulation of ECR plasma. Dougar et al presented an electrostatic model with the use of an eight-point CIC schemes to simulate the plasma confinement in a minimum-B and a zero-B traps for ion source based on the ECR phenomenon [5]. In 2004, the group of Dougar developed a Particle-in-Cell (PIC) code to simulate the heating and escaping of plasma confined to the 14 GHz minimum-B magnetic trap [6]. The microwaves injected into the chamber were treated as a multimode standing waves regime. Although electromagnetic models are complex, they are close to the real conditions of ECR plasma. Koh et al studied the ECR microwave discharge using a 1D3V electromagnetic Particle-in-Cell Monte Carlo Collision (PIC/MCC) method [7]. In the model, the electric and magnetic fields were calculated

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through Maxwell equations. Ardehali et al did the similar work, and the difference was that the propagation of electromagnetic wave in the presence of a constant external magnetic field and a linearly decreasing magnetic field were considered [8].

In the models mentioned above, electrostatic and fluid models are not appropriate to study electromagnetic characteristics of microwave. Electromagnetic particle models are suitable to describe the microscopic features of charged particles and cyclotron resonance motion of electrons. In this paper, a 1D3V PIC/MCC code is developed to simulate the microwave propagation in the plasma. Constant external magnetic fields and a mirror magnetic field are used to study the motions of electrons in the microwave plasma.

MODEL DESCRIPTION

In the 1D3V PIC/MCC code, an electromagnetic wave with frequency of 2.45 GHz feeds into the system along the z axis. The original electrons in the system are heated by absorbing the energy of microwave. When the energy of electrons is above the ionization energy of lithium, the ionization process occurs. The produced plasma is confined by external magnetic field. The ionization process is simulated by MCC, and the motion of particles in the electromagnetic field is simulated by PIC code. The flow chart of the code is shown in Fig. 2.

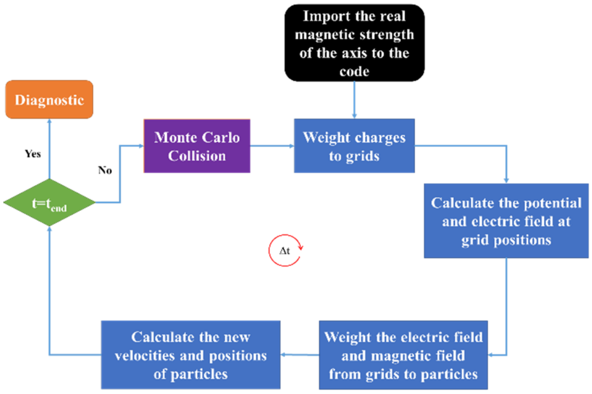

Figure 2: The flow chart of the PIC/MCC code.

The propagation of microwave

In this code, Finite-Difference Time-Domain (FDTD) method is used to simulate the propagation of 2.45 GHz microwave on a spatially discretized mesh. According to Maxwell Eq. (1) and (2), the transformation form (3) to (8) with the assumption that the fields of microwave have no variation in x and y direction can be deduced.

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} \tag{2}$$

$$\frac{\partial E_y}{\partial z} = \frac{\partial B_x}{\partial t} \tag{3}$$

$$\frac{\partial E_x}{\partial z} = -\frac{\partial B_y}{\partial t} \tag{4}$$

$$\frac{\partial B_z}{\partial t} = 0 \tag{5}$$

$$-\frac{\partial B_y}{\partial z} = \mu_0 J_x + \frac{1}{c^2}\frac{\partial E_x}{\partial t} \tag{6}$$

$$\frac{\partial B_x}{\partial z} = \mu_0 J_y + \frac{1}{c^2}\frac{\partial E_y}{\partial t} \tag{7}$$

$$0 = \mu_0 J_z + \frac{1}{c^2}\frac{\partial E_z}{\partial t} \tag{8}$$

In the equations above, E is electric field, B is magnetic field, J is current density, t is the propagation time of microwave, z is the coordinate of the propagation direction, μ_0 is magnetic conductivity in the vacuum and c is the velocity of light.

A circularly polarized electromagnetic plane wave enters the system at the start point with the assumption that the microwave is absorbed completely at the end of the system.

Particle-in-Cell Part

In this paper, an explicit PIC method is applied to simulate the motion of particles. The length of the system is 103.5 mm which is the real length of the plasma chamber. The system is discretized into 4403 uniform meshes. The charges of particles are distributed in the meshes. And the potential $\Phi$is calculated by Poisson equation as shown in Eq. (9) using multigrid method [9].

$$\nabla^2 \Phi = -\frac{\rho}{\varepsilon_0} \tag{9}$$

In the equation above, Φ is the potential, ρ is the charge density and $\varepsilon_0$is the dielectric constant in the vacuum.

The electric field is calculated by Eq. (10) with the method of finite difference.

$$\mathbf{E} = -\nabla \Phi \tag{10}$$

When the process above is finished, weight the electric field and magnetic field from grids to particles. Then calculate the new velocities and positions of particles using relativistic Boris method [10]. When the charged particles collide with the boundaries, they will be absorbed immediately. Constant magnetic fields and mirror field are used in the code.

Monte Carlo Collision Part

The null collision method is used [11] to perform the Monte Carlo Collision in our simulation. As shown in Eq. (11), a maximum collision frequency in space and energy is defined.

$$\nu_{max} = \max_{\mathbf{x}}\left(n_t(\mathbf{x})\right) \max_{\varepsilon}\left(\sigma_T(\varepsilon) v\right) \tag{11}$$

In the equation above, n_t is the number density of the particles and σ_t is the cross section of reaction.

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When ν_{max} is got, a total collision probability which is independent of particle energy and position is calculated according to Eq. (12).

$$P_T = 1 - exp(-\nu_{max}\Delta t) \qquad (12)$$

$N_c = P_T N$ particles in the particle list are chosen randomly, and a random number $0 \le R \le \nu_{max}$ is selected to determine the type of collision for each particle.

RESULTS AND DISCUSSION

In order to validate the PIC code, the two stream instability process is performed and compared with the results got by Birdsall [12]. Two opposing streams of charged particles with a perturbation in their density are unstable. Two streams of particles with the same mass charge ratio are loaded in the system, and the velocities of the two streams are set as $v_x = 1$ and $v_x = -1$ which are non-dimensional. The perturbation is carried out by adding a small sinusoidal perturbation in the density of the particles of each species. The boundary of the system is periodic. Figure 3 shows the comparison of our simulation results with Birdsall's. It can be seen that the results show good agreement with those from Birdsall, which validates the PIC part of our code.

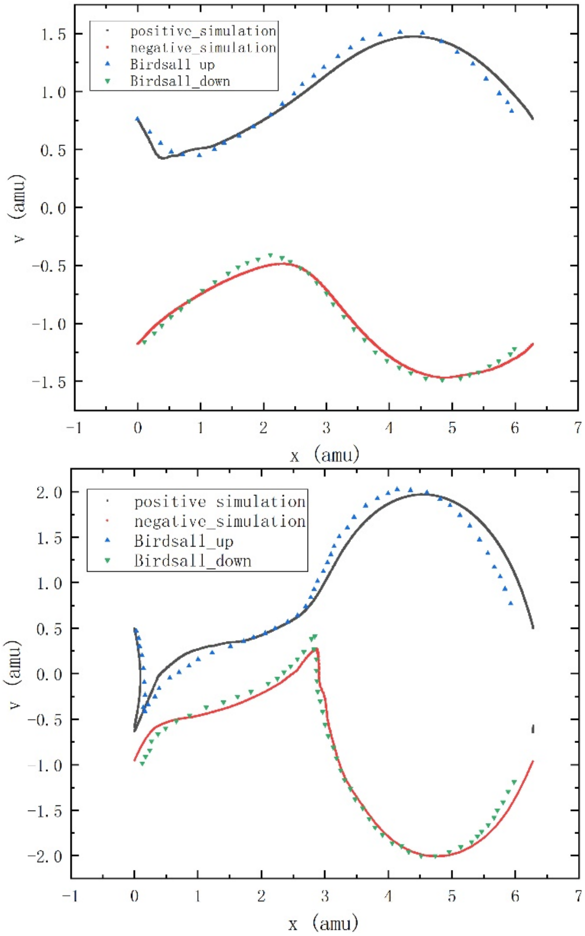

Figure 3: The phase space plots of two stream instability (up figure: t = 16, down figure: t = 18).

Figure 4 presents the profiles of transverse wave electric field E_y in different magnetic fields. When there are no particles and external magnetic field in the system, the microwave propagates along the axis in a shape of perfect sinusoidal wave. It confirms the validation of the propagation of microwave of the code. When the external magnetic field is 875 G which corresponds to the resonant magnetic field of 2.45 GHz microwave, the profile of E_y shrinks nearly around the zero line. It means that the energy of microwave is strongly absorbed by particles mainly electrons in cyclotron resonance conditions. When the magnetic field is changed to 1875 G, the resonant magnetic field of 5.25 GHz microwave which is much larger than the frequency of the incoming microwave, the profile of E_y damps slightly, which indicates that the microwave can propagate the plasma fluently.

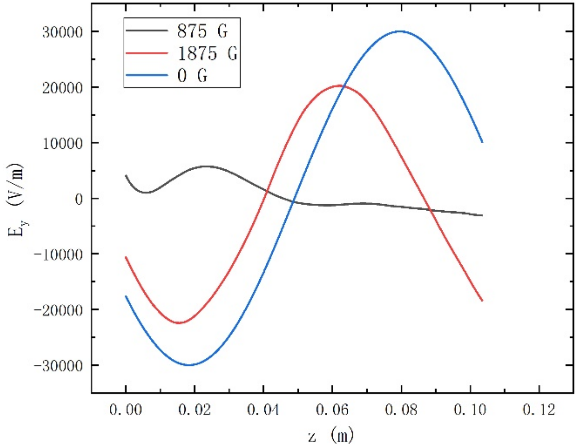

Figure 4: Profiles of transverse wave electric field E_y in different external magnetic fields.

Figure 5 shows the profiles of transverse wave electric field E_y in constant magnetic field and mirror field. The green line represents the strength of mirror field. It is apparent that within the first 40 mm in the axial direction, the strength of mirror field declines and the profile of E_y in mirror field gets close to the zero line faster than the profile of E_y without plasma. After 40 mm, the strength of mirror field arrives at the lowest point and starts to get through the second peak and the profile of E_y in mirror field oscillates around the zero line with smaller amplitude compared with the profile of E_y without plasma. Compared with the profile of Ey in constant 875 G magnetic field, the energy of microwave is absorbed dramatically at the valley of the mirror field.

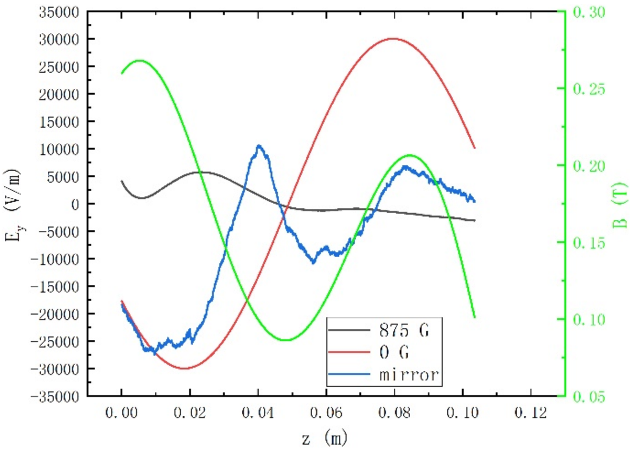

Figure 5: Profiles of transverse wave electric field E_y in constant external magnetic field and mirror field.

Figure 6 displays the v-z phase space distribution of electrons within the mirror field. There is a significant increase of the transverse velocities of electrons at the valley of the mirror field. This phenomenon corresponds to the results of Fig. 5 that the electrons are confined at the valley of the mirror field and absorb the energy of microwave propagating at this area. The axial velocities of electrons do not show any particular change.

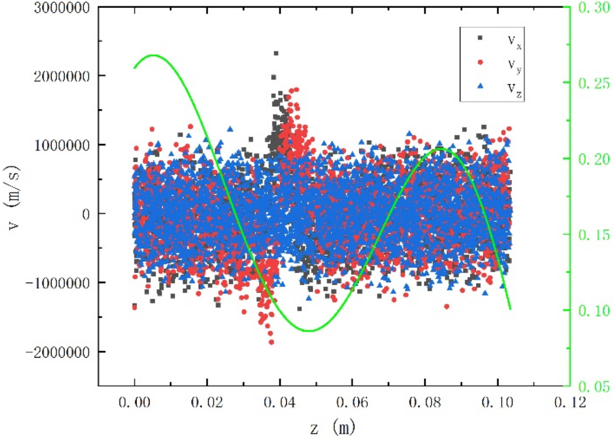

Figure 6: v-z phase space distribution of electrons within the mirror field.

The simulation results indicate that the coupling of the external magnetic field of 875 G and 2.45 GHz microwave can make the microwave lose almost all its energy to the plasma. Electrons trapped in the mirror field absorb the energy of the microwave effectively, gaining their transverse velocities.

SUMMARY AND PROSPECT

A 1D3V PIC/MCC code is developed to simulate the propagation of 2.45 GHz microwave in lithium plasma with constant magnetic field and mirror field and the v-z phase space distribution of electrons within the mirror field is also studied. The simulation results show that the energy of microwave is absorbed significantly when the external magnetic field is 875 G. Electrons trapped in the mirror field can dramatically absorb the energy of microwave, leading to the increase of the transverse velocities. The motion of electrons in mirror field is meaningful for us to understand the physics of the lithium ion source.

In the future, the behaviour of lithium ions will be considered, including the charge state distribution, the ionization rate, the influence of the density of lithium vapour and so on. All these researches are in progress, and will be reported later.

ACKNOWLEDGEMENTS

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REFERENCES

[1] J. F. Zhang et al., “Preliminary design of a hybrid ion source for $^7Li^{3+}$ generation”, presented at ICIS’17, Geneva, Switzerland, Oct 2017, paper T3Mo43, unpublished.

[2] A. Girard *et al.* “Modeling of electron-cyclotron-resonance-heated plasmas”, *Phys. Rev. E*, vol. 62, p.1182, 2000, `grl=43144362Sk|vUhyH195144;5`

[3] H. Muta *et al.* “Three-dimensional simulation of microwave propagation in an electron cyclotron resonance plasma”, *Jpn. J. Appl. Phys.*, vol. 36, p.4773, 1997, `grl= 43144462jjap16914776`

[4] D. H. Edgell et al. “Modeling of electron cyclotron resonance ion source plasmas”, in *Proc. PAC’01*, Chicago, USA, Jun. 2001, pp. 2135-2137, `grl= 43144392pac1533419;7634`

[5] V. D. Dougar-Jabon *et al.* “Plasma confinement in an electron cyclotron double cusp trap”, *Phys. Scr.*, vol. 62, p.183, 2000, `grl= 431456;2pk|vlca1rhgular1395a334;6`

[6] V. D. Dougar-Jabon *et al.* “Properties of plasma in an ECR minimum-B trap via numerical modeling”, *Phys. Scr.*, vol. 70, p.38, 2004, `grl= 431456;2pk|vlca1rhgular1373a3336;`

[7] W. H. Koh *et al.* “Electromagnetic particle simulation of electron cyclotron resonance microwave discharge”, *J. Appl. Phys.*, vol. 73, p.4205, 1993, `grl= 4314396241655;55`

[8] M. Ardehali, “Simulation and analysis of electron cyclotron resonance discharges”, arXiv preprint physics/9810033, 1998.

[9] J. H. Ferziger and M. Peric, *Computational methods for fluid dynamics*. Berlin, Germany: Springer, 2012.

[10] J. P. Boris, “Relativistic plasma simulation-optimization of a hybrid code”, in *Proc. 4th Int. Conf. on Numerical Simulation of Plasmas*, 1970, pp.3-67.

[11] V. Vahedi and M. Surendra, “A Monte Carlo collision model for the particle-in-cell method: applications to argon and oxygen discharges”, *Comput. Phys. Commun.*, vol. 87, p.179, 1995, `grl=431434923343-4955(94)33474-w`

[12] C. K. Birdsall and A. B. Langdon, Plasma physics via computer simulation, New York, USA: IOP Publishing Ltd, 1991.