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Numerical study on sheath formation near materials using Particle-In-Cell simulation

Nghiên cứu số về sự hình thành lớp vỏ bọc điện thế gần bề mặt kim loại sử dụng phương pháp mô phỏng Particle-In-Cell

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Abstract

The sheath formation in front of the wall has been studied by applying the Particle-In-Cell (PIC) method. This method is based on the particle transport to simulate the field quantities. The model consists of the flow of electrons and ions, flowing continuously into the simulation box. The source sheath and the collector sheath are found at the equilibrium stage, which are within several Debye lengths. The simulation results are in agreement with the theoretical studies, leading to a further application of the code for the plasma edge study.

Keywords: sheath formation; Particle-in-Cell model; electric potential.

Tóm tắt

Báo cáo này nghiên cứu về sự hình thành của lớp vỏ bọc điện thế ở trước bề mặt kim loại bằng phương pháp mô phỏng Particle-in-Cell. Đây là phương pháp được xây dựng dựa trên sự chuyển động của các hạt plasma để tính toán các trường vật lý có trong hệ. Mô hình này bao gồm các hạt electron và ion có dòng chảy được duy trì liên tục trong hệ. Lớp vỏ bảo vệ nguồn hạt và bảo vệ điện thế gần bề mặt kim loại được hình thành khi hệ đạt trạng thái cân bằng, có độ dày bằng vài lần kích thước Debye. Kết quả mô phỏng cho thấy sự tương đồng với kết quả được tính toán bằng lý thuyết, mở ra một tầm nhìn mới cho việc áp dụng mô hình này trong những nghiên cứu về vùng rìa tokamak sau này.

Từ khóa: sự hình thành bỏ học điện thế; mô hình Particle-in-Cell; điện thế.

1. Introduction

In magnetically confined fusion plasmas, the temperature of the core plasma is extremely high, approximately 100-200 million degrees Celsius. This temperature is much higher than any melting point of all metals. The plasma core, therefore, must be separated from the first wall

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materials as far as possible [1]. The magnetic field lines are closed in the core region to keep the plasma in a certain volume. In the edge region, the magnetic field lines are opened. Highly energetic particles can leave the confined plasma and attach the surrounding materials along these opened magnetic field lines. These phenomena cause two important issues for fusion research. First, the plasma bombards the materials at the divertor directly, so the lifetime of the first wall's materials might reduce considerably. Second, impurities eroded from the wall can enter the plasma region and degrade the core plasma performance. Therefore, the study of Plasma-Wall Interaction (PWI) is necessary for fusion research. Recently, the model that is widely used to investigate PWI is the coupling of the fluid model of the edge plasma and the kinetic model of neutrals (e.g. SOLPS package). However, the predictions from the fluids model are sometimes different from the observation. Because ions and electrons surrounding the wall have high energetic and heat fluxes, the fluid model is not perfect anymore for describing the physics properties due to the effect of kinetic ions and electrons. One of the candidates for solving this problem is using the fully kinetic description. To understand the physics behaviors of the particles in front of the wall region, the basic physics phenomenon in this region should be carefully studied as the priority. In this paper, we show how the sheath formation has been distributed at the first wall using the model based on the fully kinetic description, which is the Particle-In-Cell (PIC) simulation model. The PIC code deals with kinetics ions and electrons, helping to understand the properties of PWI, and can be used for cross-checking the fluid results derived analytically [2]. We model the flow of plasma consisting of ions and electrons in the simulation, assuming that there is no collision between these particles. How the simulation is set up and how the numerical method is applied to study the sheath formation is given in Section II. The simulation results will be discussed in the Section III. The formation of the sheath potential in front of the wall is provided in this section. The discussion and conclusion are mentioned in the last section, Section IV.

2. Simulation models

The PIC simulation is a useful tool to model the electric potential structure self-consistently, using a fully kinetic description [3]. It has been developed based on the idea of chasing the motion of each individual charged particle to simulate the behavior of plasma. The microscopic quantities including the positions and velocities of each particle are used, and all macro-quantities like density, and current density can be estimated. We considered the electrostatic case in this study in which the electric field is self-consistently calculated each time step by the charge and current densities. In contrast, the magnetic field is constant in time. The basic equations used in PIC simulation include two main groups: equations of motion and field equations. The two first-order different equations of motions of each particle are:

$$\frac{d\mathbf{x}}{dt} = d\mathbf{v}, \quad (1)$$

and

$$m\frac{d\mathbf{v}}{dt} = q(\mathbf{E} + \mathbf{v}\times\mathbf{B}), \quad (2)$$

where **x**, **v**, q, m are the particle's position, velocity, charge, and mass, respectively. **E** and **B** represent for the electric field and the magnetic field. The field equations to be solved are

$$\mathbf{E} = -\nabla\Phi, \quad (3)$$

$$\nabla\cdot\mathbf{E} = \frac{\rho}{\varepsilon_0}, \quad (4)$$

which are combined to archive *Poisson's equation*

$$\nabla^2\Phi = -\frac{\rho}{\varepsilon_0} \quad (5)$$

where Φ and ρ are the electric potential and charge density, respectively. The detail of how these equations are solved numerically and how the PIC cycles work in each time step is proposed in F. Chen's book in reference [4]. In this work, the system is considered to be in one-dimension x of space with three dimensions of velocity (v_x, v_y, v_z) (1D3V). The particle's position and velocity take all the values in **v** and **x** space. On the other hand, the field quantities will be obtained on the spacial grid, known only at discrete points in space.

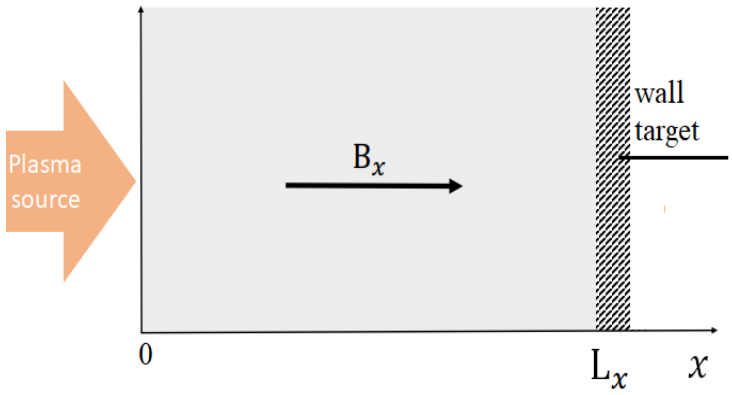

Figure 1. Simulation system. The magnetic field is constant in space. Particles enter the simulation box from the left-hand side while being fully absorbed at the right-hand side boundary where x = L_x = 0.03m.

To study the sheath formation in front of the wall, the simulation domain has been set up as in Fig. 1. At the beginning of the simulation when $t = 0$, the system is free of plasma. There is no particle in the simulation at this time. The right-hand side boundary where $x = L_x$ is considered as a wall. The wall is assumed to satisfy the floating potential condition. Particles are fully absorbed at the wall. Particles are injected during the running time of the system on the left-hand side at $x = 0$. The temperatures of the ions and electrons source have a half-Maxwellian shape. In this study, the system length is set to $L_x = 0.03m$, mass ratio $m_i/m_e = 1836$, electrons and ions have source temperatures as $kT_e = 1eV$, $kT_i = 10eV$. Since the real mass ratio between electrons and ions has been used, the results can bring a clear picture of the particle transport as in the real experiment. The plasma source density is considered to be low, which is nearly the same as Q-machine. No collision, reflection, or recycling process is considered in this study.

3. Results

Figure 2 shows values of potential at the wall (or the collector) ϕ_C at every time step from the beginning until $t = 1000$ steps are run. The potential starts with zero when there is no plasma at the initial stage. After the first several time steps, the potential ϕ_C decreases drastically. This is mainly because electrons are lighter than ions, and their thermal velocities are higher than that of the ions. Therefore, electrons go faster than ions to reach the wall. Subsequently, the number of electrons hitting the wall is larger than ions, leaving the plasma with a net positive charge. With time increases, the wall charges up. The electrons are repelled to the source, while ions are attracted to reach the wall [5]. The potential at the wall is increased and then remains stable, as displayed in Fig. 2. After 30 time steps, the potential starts increasing and from 600 time steps, it becomes stable. This stage is named the equilibrium stage when the number of ions and electrons are nearly equal in

the system. At this stage, not only the potential at the wall, but all of the other field quantities also remain constant. The plasma is still flowing into the simulation after this stage but keeps the same trend and amount each time. Therefore, stooping the simulation after 1000 time steps does not affect the results of the simulation. All of the values at any certain time will be taken time-average to reduce the noises and numerical errors.

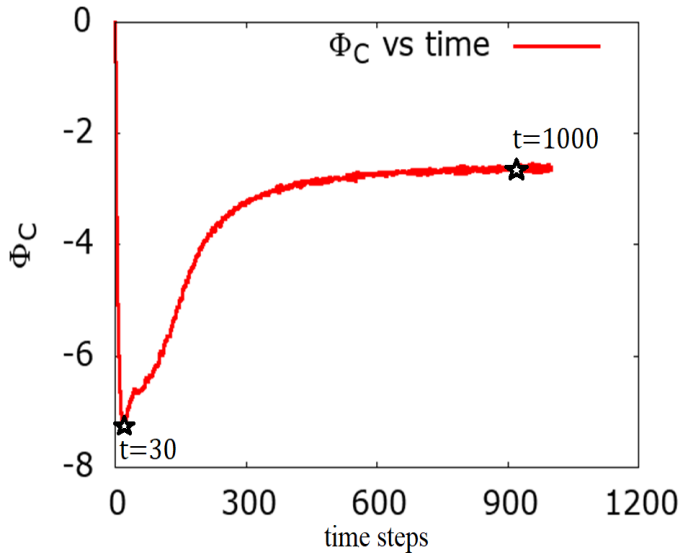

Figure 2. Time evolution of potential at the wall ϕ_C. ϕ_C drops drastically at the first time steps and increases until the simulation reaches the equilibrium stage. After this stage, the value of ϕ_C remains stable.

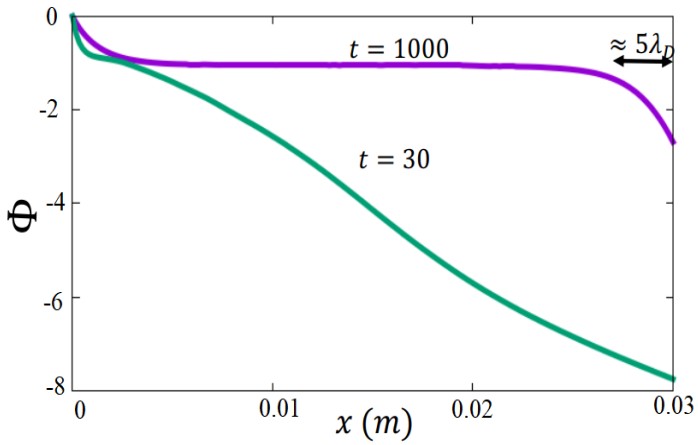

Figure 3. Potential profile in the system at 30 (as green line) and 1000 (as purple line) time steps.

The green line in Fig. 3 shows the potential at $t = 30$ time steps, where the simulation has not been in the equilibrium stage yet. At this time, the number of electrons and ions still has not been balanced. More electrons hit the wall than the ions. The potential profile is displayed as the slope line. At the equilibrium stage, most of the electrons are located near the source, and only the electrons having a high velocity reach the wall. Consequently, near the source, the number of electrons is higher than that of ions. In the middle region, the number of electrons and ions is equal, and ions are more in front of the wall than electrons. Because of this property, two sheaths have formed in the system. The source sheath is near the source of the system and the

collector sheath is next to the wall. As seen in the purple line in Fig. 3, the sheath potential has been formed within a small length near the source and the collector. For example, the collector sheath length is approximately $\approx 5\lambda_D$, where λ_D is the Debye length. These two sheaths are to protect the plasma at the middle region when the charge densities become zeros or $n_e = n_i$ [6]. For code verification, we compare our results with the theoretical analysis. Figure 4 illustrates the potential values at the wall ϕ_C and potential drop ϕ_P between theoretical analysis and the simulation results using different ion source temperatures. Here, electron source temperature $kT_{e0} = 1eV$ is used for all simulation cases. In the theoretical study, at the equilibrium stage, the fluxes of electrons and ions are constant in space, yielding

$$\frac{n_{i0}}{n_{e0}} = \left(\frac{m_i}{m_e}\frac{T_e}{T_i}\right)^{1/2} \exp\left(\frac{e\Phi_C}{kT_e}\right) \quad (6)$$

Ion and electron densities can be computed as

$$n_e(\Phi) = \frac{n_{e0}}{2}\exp\left(\frac{e\Phi}{kT_e}\right)\left[1+\mathrm{erf}\left(\frac{e\Phi - e\Phi_C}{kT_e}\right)^{1/2}\right], \quad (7)$$

$$n_i(\Phi) = \frac{n_{i0}}{2}\exp\left(-\frac{e\Phi}{kT_i}\right)\mathrm{erf}\left(-\frac{e\Phi}{kT_i}\right)^{1/2}. \quad (8)$$

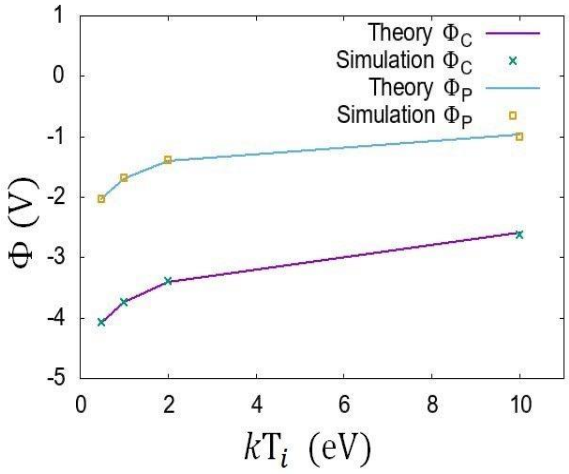

Figure 4. Comparison of potential at the wall ϕ_C and potential drop ϕ_P between theoretical analysis and the simulation results using different ion source temperatures. The simulation results are in agreement with the theoretical study.

The potential drop (i.e. $\nabla^2\phi = 0$) is the potential computed at the region where electron and ion density are equal. Our simulation results propose similar values for ϕ_C and ϕ_P as the theoretical analysis. As a result, even using the simple simulation and unrealistic input parameters, the simulation results still can be used to study the sheath formation of the potential in the magnetic devices.

4. Conclusion

The sheath near the plasma wall has been studied using PIC simulation. In a one-dimensional electrostatic case, the sheath structure of the wall is treated self-consistently with Maxwellian source ion and electron temperatures. The collector sheath is formed to protect the wall from highly energetic particles, while the source sheath is to protect the source. The obtained sheath is several Debye lengths in front of the wall. The code is verified with the theoretical analysis. The simulation results are in agreement with the theoretical analysis, giving the possibility for further studying the particle transport near the wall. The sheath potential drops at the middle region where the ions and electrons densities are equal. The formation of

the sheath could be one of the candidates to explain the electric potential profile near the first wall in tokamak using PIC simulation. Understanding sheath formation should have a strong impact on the understanding of plasma wall interaction at the first wall to avoid damage to the wall due to the transient heat fluxes near the divertor in the tokamak. This issue will be discussed in future work.

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