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Particle-in-cell/Monte Carlo simulation of plasma for inner coating of a pipe

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Abstract

A high-density plasma is generated inside a cylindrical target as a result of the hollow cathode discharge effect under a proper condition. The hollow cathode discharge plasma can be applied to the inner coating of the target. In order to analyze the plasma behavior near a cylindrical target, simulations have been carried out using the simulation software “PEGASUS” with a cylindrical coordinate system. The gas pressure was 0.1–600 Pa and a negative pulse or DC voltage (−30 eV~−20 kV) was applied to the target. RF (13.56 MHz) and a superposed voltage of DC and RF were also applied. Effects of gas pressure, secondary electron emission coefficient, and length and inner diameter on the plasma generation were studied, and Paschen-like curves for a hollow cathode discharge were obtained for both centimeter-sized and millimeter-sized pipes. Plasma generation in the surroundings of a pipe with a grounded rod on the axis was also simulated. It was found that a hollow cathode discharge plasma works only for a short pipe of length vs. diameter less than 5. For a pipe of higher aspect ratio, a glow discharge plasma between the inside wall and a rod on the axis works well regardless of the length.

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1. Introduction

By plasma immersed ion implantation (PIII), it is possible to implant and deposit coatings on complex shape surfaces of targets [1]. In addition, there is a great commercial interest in implanting and coating on the inside surfaces of pipes and holes. Sheridan [2] calculated the structure of the ion-matrix sheath in a cylindrical bore and found that the important length scale is the ion-matrix overlap radius $s_1=(4\varepsilon_0 V/en_0)^{1/2}$, where V is the voltage applied to the target and n_0 is the plasma density. The radius is $\sqrt{2}$ times the ion-matrix sheath width for the planar target. Typical values of the ion-matrix overlap radius for V=1 kV is 14.9 cm for $n_0=10^{13}$ m^{-3} and 0.47 cm for $n_0=10^{16}$ m^{-3}. However, in his calculation, “end” effects are not included since the calculation is one-dimensional. In reality, when a bore or a pipe is not so long enough, the “end” effect such as electron escape or plasma entering from the end of bore or pipe is not negligible but plays an important role in the plasma generation inside a bore or a pipe. However, it is difficult to include the “end” effect in the analytical calculation.

We have developed the simulation software “PEGASUS” [3,4] for the analysis of the behavior of ions, electrons and neutral atoms in the plasma as well as the spatial distribution of the electromagnetic field. For plasma analysis of low pressure gas, which are used in PIII and D, the software uses a particle-in-cell (PIC) method [5,6] for the analysis of electromagnetic fields and movement of charged particles. A Monte Carlo collision (MCC) method [7,8] is used for collisions of ions, electrons, and neutrals in the plasma, and

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the dynamic-SASAMAL code [9,10] is used for the ion–solid surface interactions. By using the PIC–MCC method, not only trajectories of charged particles in the electromagnetic field but also the behavior of non-equilibrium low temperature plasmas can be simulated [7].

In order to obtain the condition for a hollow cathode discharge, PIC–MCCM simulations have been performed. Hollow cathode discharges occur at lower voltages and carry orders of magnitude higher currents than ordinary glow discharges of similar dimensions and gas parameters. Using PEGASUS, plasma generations in Ar gas in surroundings of a cylindrical target of centimeter-sized and millimeter-sized in radius, to which a pulsed-, a DC-, or an RF+DC-negative voltage was applied, have been simulated under various conditions in length, gas pressure, voltage, and secondary electron emission coefficient. Paschen-like curves for the follow cathode discharges were obtained for a pipe of both centimeter- and millimeter-sized in radius, which were compared with the ordinary Paschen curve for the glow discharge between planar electrode. Plasma generation in surroundings of a cylindrical target with a grounded rod on the center axis was also simulated.

2. Simulation model

The outline of the PEGASUS was given in Refs. [3,4], so only a brief outline is presented here. In the PIC method, individual particles are not followed in order to reduce the computation time. Instead, movements of super particles are followed. A super particle is a bunch of charged particles of the same kind. So, the charge and the mass of a super particle may be 10^8 to 10^{10} times those of the real particle depending on the statistical condition. The collision rates are calculated based on the energy-dependent cross section. The particle energy is calculated from the electromagnetic field, which is obtained from Poisson's equation using the densities of charged species.

The Nouman boundary condition is applied to the open boundary. To the target, a fixed potential is set (pulsed, DC, RF, or superposition of them) and the chamber wall is grounded.

In a real hollow cathode discharge condition, when the discharge starts and the target current intensity starts increasing, the applied voltage decreases to some level following the power limit of the system. Then, the target current is kept on a limited level. However, such an effect is not included in PEGASUS so far. Hence, in the simulation, when hollow cathode discharge starts, the plasma density increases without a limit.

Fig. 1 shows the schematic arrangement of target and anode. The time dependence of applied pulse voltage to the target is shown in the inlet graph. A two-dimensional cylindrical coordinate system was used. The system is symmetric to the x- and y-axis, so only one quarter was simulated. Neumann boundary conditions were used on the x- and y-axis. Calculations were carried out for Ar gas pressures of 0.1–600 Pa, with an applied voltage of 30 V to 20 kV. The initial plasma density is 10^{13} m^{-3} with initial number of super particle of 10 000, in general. With an initial plasma density lower than 10^{13} m^{-3}, the calculation consumes longer time and the obtained results are almost the same.

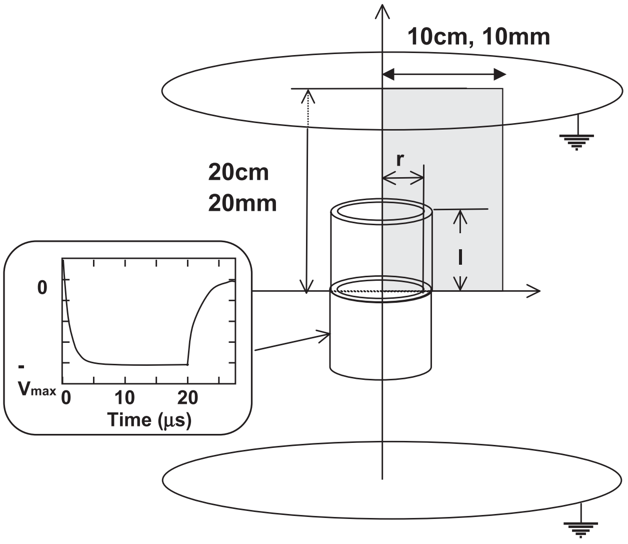

Fig. 1. Schematics of the simulated system: cylindrical target and planer anode. The pulse shape of applied voltage is shown in the inset graph.

3. Results and discussions

When a negative voltage is applied to a cylindrical target, a hollow cathode discharge, or a glow discharge, or no plasma generation occurs depending on the gas pressure, the applied voltage, and the secondary electron emission coefficient (γ). Fig. 2 shows simulation results for a pipe 2 cm in radius and 10 cm in length in Ar gas. In this case, a negative pulse voltage (pulse length: 20 μs) was applied to the target. However, the discharge starts before the pulse reaches the end, so that there is no difference between the simulation results obtained with a pulse voltage and a DC voltage except for a time to the discharge. Under the conditions of 50 Pa–3 kV (a) and 10 Pa–200 V (b), a hollow cathode discharge plasma generates. When a negative voltage is applied to the target, electrons move off the target quickly, and as a result, plasma is generated by electron collisions with gas atoms between the pipe edge and the anode. The place where the most intense plasma generates is near the center axis just above the pipe end. Then, the plasma goes into the pipe. Finally, pendulum motion starts and hollow cathode plasma generates [11,12]. When the pressure is too high, discharge does not occur with a low voltage, and a glow discharge occurs with a high voltage ((c) 100 Pa, −1 kV). When the pressure is too low, a plasma does not generate with a low voltage and a discharge starts outside of the pipe with a high voltage ((d) 2 Pa, −1 kV). Fig. 3 shows