Particle-in-Cell Simulation of Ion Flow Through a Hole in Contact With Plasma

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Abstract—Images from a particle-in-cell (PIC) simulation of ion flow through a hole in contact with plasma are presented. When the hole size is comparable to or larger than the plasma sheath thickness, the emanating ion beam is strongly divergent. In the opposite extreme of small hole size, a collimated ion beam may be extracted.

Index Terms—Ion angular distribution, ion beams, particle-incell, plasma molding, simulation.

ON extraction through a grid finds applications in ion beam as well as neutral beam sources. The energy and directionality of the extracted beam are critical for such applications. Anisotropic etching of microelectronic materials, for example, requires a well-collimated beam. For an otherwise flat grid, the angular distribution of the extracted beam depends primarily on the diameter of the gird holes, D, as compared to the plasma sheath thickness, $L_{\rm sh}$. When $L_{\rm sh} \gg D$, the plasma-sheath interface (meniscus) is essentially planar as if the holes were not there (e.g., a solid wall). In the other extreme, $L_{\rm sh} \ll D$, the plasma "leaks" through the holes. In the intermediate case, $L_{\rm sh} \sim D$, the plasma-sheath meniscus "bends" gently over the holes [1]. The resulting beam should be highly directional (assuming no collisions in the sheath) when $L_{\rm sh} \gg D$, and highly divergent when $L_{\rm sh} \ll D$. On the other hand, the energy of the beam will depend on the plasma potential.

In this work, a particle-in-cell (PIC) simulation was used to study the angular and energy distributions of an ion beam extracted from a radio frequency (RF) plasma. A single hole in contact with the plasma was considered as a simple geometry simulating a grid hole. Two hole diameters (508 and 50.8 μ m) in a 254- μ m-thick conductor plate were considered. The computational domain (only part of it is shown in Fig. 1) extended sufficiently far from the hole to avoid edge effects. The ion density $(n_{i0} = 3 \times 10^{11} \text{ cm}^{-3})$, electron temperature $(T_e = 6.8 \text{ eV})$, and RF potential ($V_0 = 40 + 20 \sin 2\pi f t$, f = 13.56 MHz), were specified at the top boundary of the computational domain. These conditions correspond to one of the experiments described in [2]. The wall containing the hole was conductive at ground potential (V = 0). A zero potential gradient condition was applied at the left, right and bottom boundaries of the computational domain. An electropositive argon plasma containing a single ion species and electrons was simulated. Only the ions were followed by PIC. The electron density was assumed to be

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Fig. 1. Time-average potential for $508-\mu$ m-diameter hole.



Fig. 2. Ion angular distribution for $508-\mu$ m-diameter hole.

given by the Boltzmann relation. The plasma sheath evolved self-consistently according to the specified conditions. The pressure (5 mtorr) was sufficiently low for the ion flow to be collisionless. The results shown below were obtained with 3×10^5 simulation particles. Particles injected at the top boundary of the computational domain were weighted according to their radial



Fig. 3. Time-average potential for $50.8-\mu$ -diameter hole.

position so that a radially uniform ion flux was injected. Particle distribution functions were collected at the bottom boundary of the computational domain. A leap-frog time integration scheme was used and the Poisson equation was solved at each time step using a finite element method. Time marching continued until a periodic steady-state was achieved. Computations were performed on a 3.2-GHz Pentium 4 personal computer. Results were visualized using Tecplot 10.0 (Amtec Engineering Inc., Bellevue, WA).

Fig. 1 shows the time-average electric potential profile for the 508- μ m-diameter hole. For the conditions examined, the time-average sheath thickness over a flat solid wall would be about 150 μ , smaller than the hole diameter. Therefore, the plasma–sheath interface "dips" inside the hole. Ions experience a strongly diverging electric field which "spreads" the extracted ion beam over large angles from the hole axis. The ion beam divergence can be clearly seen by plotting the ion angular distribution (IAD) (Fig. 2). The predicted distribution is similar to that found experimentally [2], taking into account that the experimental IAD was cut off at about 35° because of shadowing. When the hole size (50.8- μ m diameter) is smaller



Fig. 4. Ion angular distribution for $50.8-\mu$ -diameter hole.

than the sheath thickness (Fig. 3), the extracted ion beam is much more collimated (Fig. 4). In this case, ions are accelerated for most of their transit through the sheath by a vertical electric field. Thus, ions acquire significant vertical velocity before entering the hole, where they "feel" a horizontal field component (divergent field) for a relatively short time. Some ion divergence is still present, however, as the IAD spreads beyond that of the incoming ions.

In summary, in plasma or beam extraction through a grid, when the grid hole size is comparable to or larger than the local sheath thickness, the resulting ion beam is strongly divergent. Collimated beams of rather uniform flux may be extracted when the grid hole size is much smaller than the local sheath thickness.

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