

# Particle-in-Cell Simulation of a Neutral Beam Source for Materials Processing

Min Sup Hur, Sung Jin Kim, Ho Seung Lee, Jae Koo Lee, *Member, IEEE*, and Geun-Young Yeom

**Abstract**—Neutral beam processing is being considered as a new technique to reduce plasma-induced damage in materials processing. We report on particle-in-cell simulations of a neutral beam source. The system is composed of an ion-beam source and multireflectors which neutralize incident ions and reflect neutral particles. It is revealed from the simulations that about 2.8% of the ion-current from an ion-beam source is successfully neutralized before reaching a diagnostic plate.

**Index Terms**—Neutral beam source, particle-in-cell simulation, plasma materials processing.

PLASMAS ARE widely used in materials processing. However plasma-process-induced damage (PPID) is becoming a more serious problem as the feature size decreases. One of the most important types of PPID is gate-oxide damage caused by the imbalance of charge accumulation on high-aspect ratio structures during semiconductor device manufacturing [1].

One of the most promising methods to overcome PPID and other charge-induced problems is using a neutral beam for etching or deposition processes. Energetic neutral particles can be made by a variety of methods, among which surface neutralization of ions is known to have the best properties [2]. Fig. 1 shows a neutral beam source which is composed of multireflectors and an ion-gun. Ions ejected from the ion-gun drift to the reflectors to be neutralized and reflected.

The characteristics of the neutral beam are determined mostly by the neutralization and reflection processes on the reflectors, as the density and velocity distribution of neutrals reflected from the reflectors depends on those of the incident ions. Therefore, it is important to simulate the motion of ions simultaneously with those of neutrals. In many simulations, only the neutral transport in the fixed plasma background is considered.

To simulate ion and neutral transport, we use the particle-in-cell (PIC) code OOPIC [3]. A new boundary condition for the reflector has been added to the OOPIC code to simulate neutralization-reflection processes. We used another code, TRIM [4], to obtain the reflection energy, angular distribution, and reflection coefficient of neutrals for various energies and angles of incident ions. Silicon is used as reflectors which

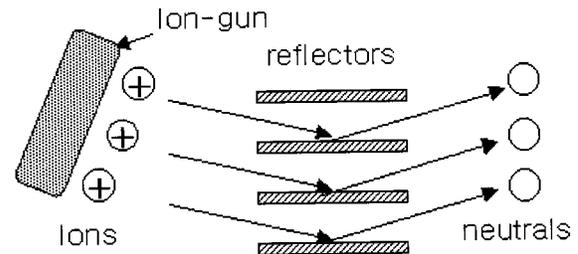


Fig. 1. Neutral beam source with multireflectors.

can be replaced by other materials with higher reflection coefficients as, and when, necessary. The reflection coefficient of argon ions on silicon obtained from TRIM is about 0.5 for an incident angle of  $75^\circ$  and incident energy of 300 eV. This value decreases as the incident angle and energy decrease. We tabulate these data to be referred to by OOPIC when ion-surface collisions occur.

Fig. 2(a) is a snap shot of a particle distribution. We obtain data from OOPIC and post-processing the data has been done by a commercial graphic package, SURFER. The ion flux of the ion-gun is  $1.39 \times 10^{17} \text{ m}^{-2}/\text{s}$  and the angle between the ion-gun-direction and the reflector-normal is  $75^\circ$ . The initial ion energy is 400 eV. Since initial ion trajectories are altered by the mutual Coulomb forces, some ions directly reach the diagnostic plate without having a collision with the reflectors. Since the reflection angle is not the same as the incident angle but has a distribution, some neutrals from the surface experience multiple reflections and mostly are lost due to implantation or deposition. The maximum neutral flux on the diagnostic plate is  $3.9 \times 10^{15} \text{ m}^{-2}/\text{s}$  which is about 2.8% of the initial ion flux [see Fig. 2(b)]. The ion-neutral conversion rate can be greatly increased by optimizing the reflector material, reflectors' width or gap, ion-beam quality, and other parameters. The length of uniform flux region on the diagnostic plate is about 0.01 m which can be improved by increasing the ion-gun's cross-sectional area. Fig. 2(c) and (d) are a space-angle distribution and a space-energy distribution of neutral velocities on the diagnostic plate. The neutral energy is concentrated near 10 eV which is 2.5% of initial ion energy. The incident angles of neutrals on the diagnostic plate are mostly between  $5^\circ$ – $20^\circ$  which is nearly the same range as the angle between the ion-gun and reflectors. This implies that the anisotropy of the neutrals is very high, which is one of the most important requirements in processing. Fig. 2(e) and (f) represent number densities of ions and neutrals.

In conclusion, we have simulated a neutral beam source model using multireflectors with a PIC code. Since the detection of neutral fluxes is more difficult than that of ions,

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M. S. Hur, S. J. Kim, H. S. Lee, and J. K. Lee are with the Department of Electrical Engineering, POSTECH, Pohang 790-784, South Korea (e-mail: jkl@postech.ac.kr).

G.-Y. Yeom is with the Department of Materials Engineering, SungKyunKwan University, Suwon 440-746, South Korea.

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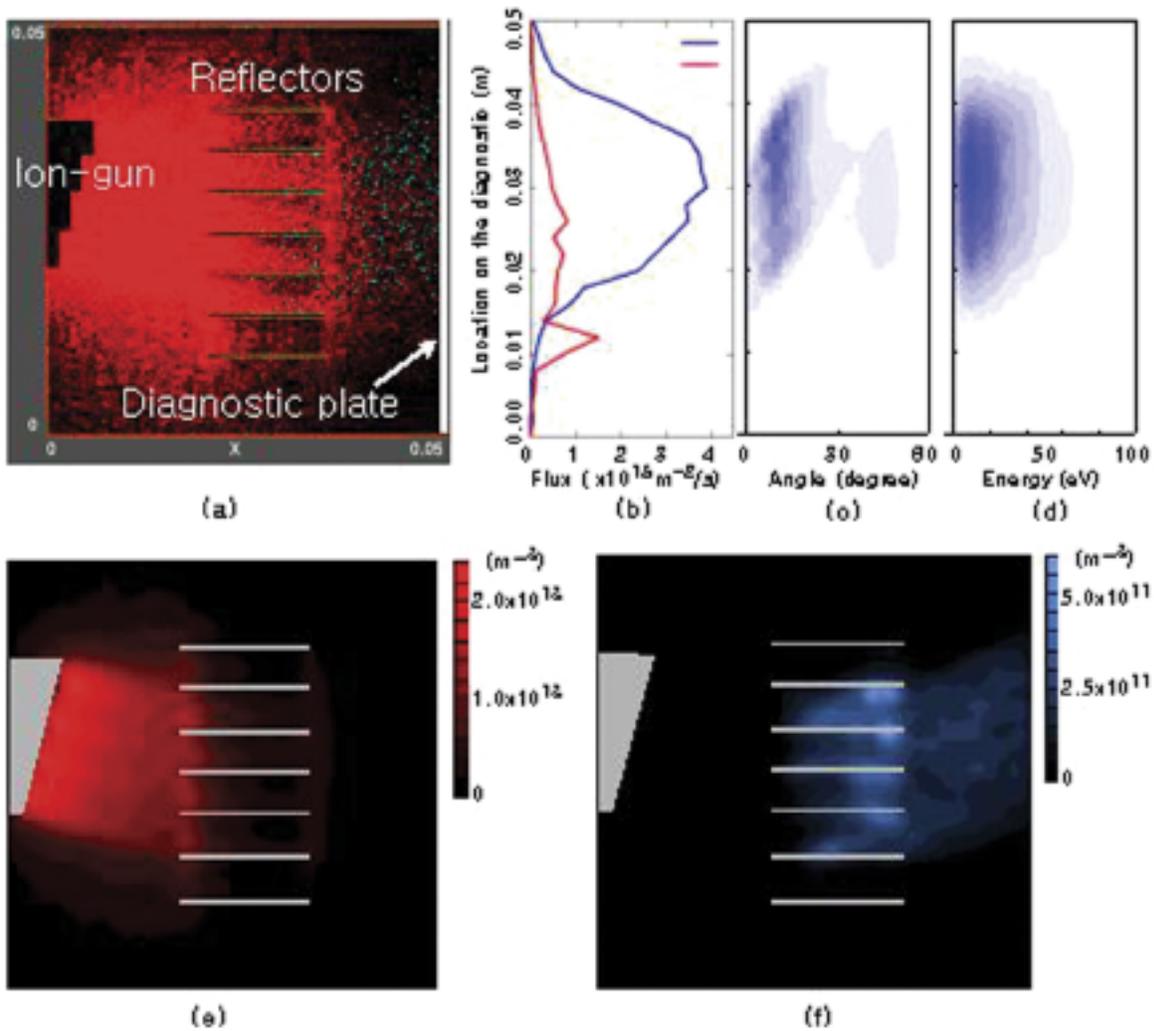


Fig. 2. (a) A snap shot of the PIC simulation for ion beam and neutral transport. The red and blue spots are ions and neutrals, respectively. (b) Comparison of ion and neutral fluxes normal to the diagnostic plate. (c) Space-angle distribution of neutrals incident on the diagnostic plate. The vertical axis is the location on the diagnostic plate and the horizontal axis is the angle between neutral velocity and the normal of the plate. (d) Space-energy distribution of neutrals incident on the diagnostic plate. The vertical axis is same as in (c) and the horizontal axis is the neutral energy. (e) Ion density and (f) the time-averaged neutral density.

simulations may come handy in studying neutral transport properties.

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