Effect of Surface Structure upon Particles Reflection Coefficients and Sputtering Yields

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The angle and energy distributions of reflected particles have been measured for pyrolytic graphite bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal. The measured angle distribution of the reflected ions is broader compared with that predicted by a Monte Carlo code ACAT for a flat surface. The surface structure of pyrolytic graphite is observed by a scanning electron microscope (SEM). The SEM image has shown the surface of pyrolotic graphite is rough and bumpy. In order to describe the surface structure of the pyrolytic graphite, the fractal surface model has been employed into ACAT. The ACAT calculations with the fractal surface model indicate a sharp angle distribution of the reflected ions are suppressed by including the surface roughness.

Keywords: reflection, sputtering, surface structure, fractal geometry, Monte Carlo simulation

1. Introduction

The beam-material interaction for a rough surface differs from those for flat surfaces. A number of Monte Carlo codes have been developed to analyze ion-solid interactions [1][2] and reproduce experimental data, such as sputtering yields [3][4], with fair accuracy. Several computer works have been done by considering the surface structure of the target material. Ruzic *et al*. have estimated the influence of the rough surface for sputtering yields by incorporating one-dimensional fractal topography into TRIM.SP [5]. Küstner *et al*. have investigated the influence of the surface structure for the incident angle dependence of sputtering yields, using data of the surface structure measured by scanning tunneling microscope (STM) and a distribution of local angles of incidence for the incident ions in TRIM.SP calculations [6]. The secondary electron emission from the bowl-structured surface is reported by Kawata and Ohya [7].

We have started experimental investigation upon how the carbon surface nanostructure affects the particle reflection and sputtering processes [8]. Recently, the angle and energy distributions of reflected particles have been measured for highly oriented pyrolytic graphite (HOPG) bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal.

In the present work, a Monte Carlo code ACAT [2] based on the binary collision approximation is adopted to simulate the influence of surface micro structure upon particle reflection and sputtering. The fractal surface model [9] is applied to describe the structure of rough surface of the target material for ACAT. The surface structure is described with the fractal dimension D which is between 2.0 and 3.0 in this model.

To quantify the effect due to surface structure of the target material the dependence of particle reflection coefficient and that of sputtering yield upon fractal dimension are calculated with ACAT. The angle distributions for fractal surfaces are broader compared with those for flat surfaces at oblique incidences. The surface geometry of the carbon target is investigated with a scanning electron microscope. The correlation of the results between the experiment and the ACAT calculation is discussed.

2. ACAT code

The ACAT code was developed to simulate the atomic collisions in an amorphous target based on the binary collision approximation. The target atoms are randomly distributed in each unit cubic cell of which the lattice constant is $R_0 = N^{-1/3}$, where N is the atomic density of the target material. The surface model in the standard ACAT corresponds to the flat surface. In the present work, in order to analyze the influence of the surface structure of the target material, the two-dimensional fractal surface model [9] (Fourier filtering method) is incorporated into the ACAT code with the periodic boundary condition. The incident position where the first collision between the incident ion and the target atom takes place and the azimuthal angles of incidence are determined from random numbers.

In the Fourier filtering method, the height z at a horizontal position $\boldsymbol{r} = x\boldsymbol{i} + y\boldsymbol{j}$ is given by the

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two-dimensional discrete inverse Fourier transform as

$$z(\mathbf{r}) = \sum_{k_x=0} \sum_{k_y=0} \{A(\mathbf{k})\cos(\mathbf{k}\cdot\mathbf{r}) + B(\mathbf{k})\sin(\mathbf{k}\cdot\mathbf{r})\}, \qquad (1)$$

where $\boldsymbol{k} = k_x\boldsymbol{i} + k_y\boldsymbol{j}$ is a wave vector. The spectral density $S(\boldsymbol{k})$ expressed by

$$S(\mathbf{k}) = A^2(\mathbf{k}) + B^2(\mathbf{k}) \propto (k_x^2 + k_y^2)^{-\beta}, \qquad (2)$$

and $\beta = 4 - D$, where D is the fractal dimension.

3. Results and discussion

Figure 1 shows the surface structure of HOPG by a scanning electron microscope. The picture indicates that the surface structure of HOPG differ from the flat surface.

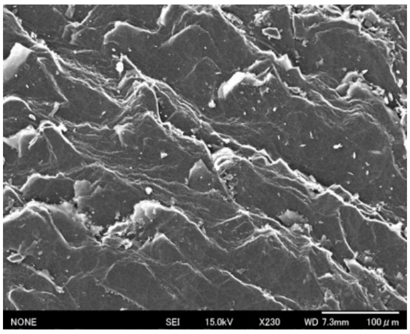

Fig. 1 SEM image showing surface structure of HOPG.

Shown in Fig. 2 is the surface structure described by the fractal method with D=2.3. In the present work, the fractal dimension 2.3 has been employed to represent the surface structure of HOPG. The fractal surface is also complex.

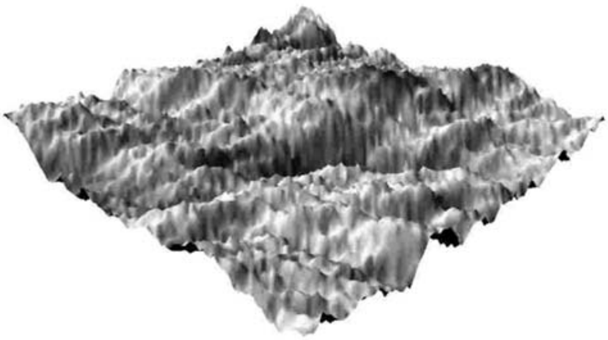

Fig. 2 Fractal surface with fractal dimension 2.3.

The angle and energy distributions of particles reflected from HOPG surface due to H^+ incidence have been measured by the experimental apparatus installed at National Institute for Fusion Science [10].

Figure 3 indicates the measured intensities of H^- and H^+ reflected from HOPG bombarded by 1 keV H^+ at the 80 degree incident angle. Also shown in Fig.3 are the ACAT results for flat and fractal surfaces. The ACTA results do not take into account of the charge states of outgoing particles, but are the net results containing positive, negative charge states and neutrals. Assuming the charge state distributions of the reflected particles have weak dependence on the reflection angles [11], the ACAT results can be directly compared to experimental data of H^- and H^+. The flat ACAT results indicate the sharp peak abound the mirror angles. Meanwhile, the reflected angle dependence of the experimental data is weaker than the dependence predicted by the flat ACAT results. For the case of rough surface, the effective incident angles has to be determined from local incident angles, β and β', distributed across the entire surface as shown in Fig. 4 [6][12]. The rough surface result obtained from ACAT calculation with incident angle distribution yields a broader distribution in agreement with the experimental data.

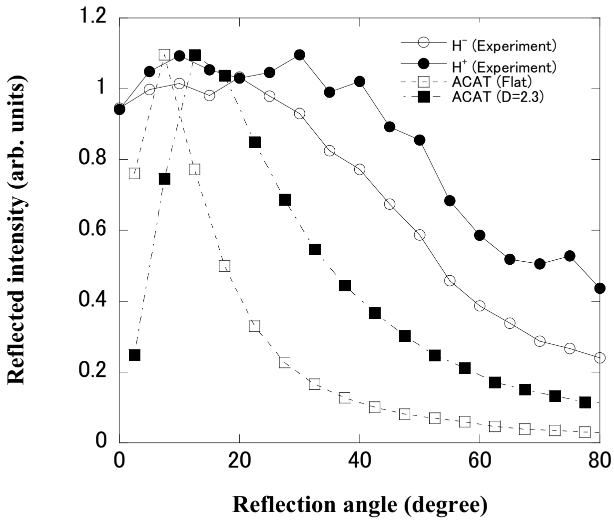

Fig.3 Measured reflected H^- and H^+ intensities bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal. Also shown in the figure are the results calculated the flat and the fractal ACAT.

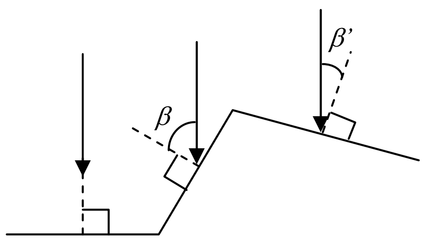

Fig. 4 Schematic representations of local angles in the rough surface.

Figure 5 indicates the measured energy distributions of the reflected ions together with the flat and the fractal

ACAT results. This indicates that the energy of reflected ions decrease with increasing reflection angle, because the ions reflected by larger angles experience some collisions with the target atoms in the solid. The large difference of the flat and the fractal ACAT is not found. The simulation by a fractal dimension of surface structure of the target material is an effective tool for the distribution of the reflected ions.

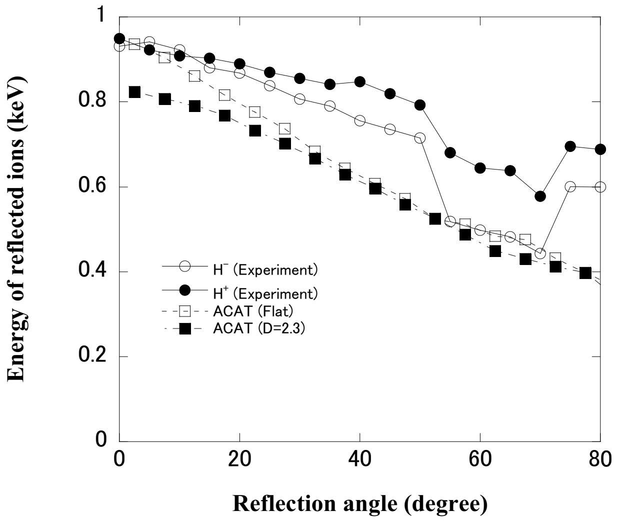

Fig. 5 Measured reflected H^- and H^+ energy distributions bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal. Also shown in the figure are the results calculated the flat and the fractal ACAT.

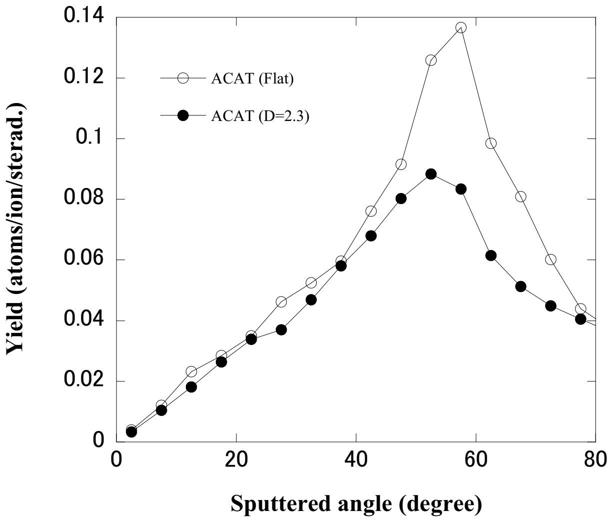

Fig. 6 Distributions of sputtered atoms calculated by the flat and the fractal ACAT under 1 keV H^+ ions bombardment at an incident angle 80 degree from surface normal.

Shown in Fig. 6 are the yields of sputtered carbon atoms bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal calculated by the flat and the fractal ACAT. This indicates that the peaks of the distributions are around at 60 degree. These angles are larger than those of reflected ions. The reason why sputtered atoms have large peak angles is that the target atoms are sputtered by collision cascades in the solid. In other words, almost of all reflected ions are reflected by few collisions. Thus, the reflected ions have the peak around the mirror angle. The angle dependence of sputtered atoms is also suppressed with the rough surface.

The energies of sputtered atoms calculated by ACAT are shown in Fig. 7. The energies of sputtered atoms are smaller compared with those of the reflected ions. The collision cascade in the target material results in the energies of sputtered atoms.

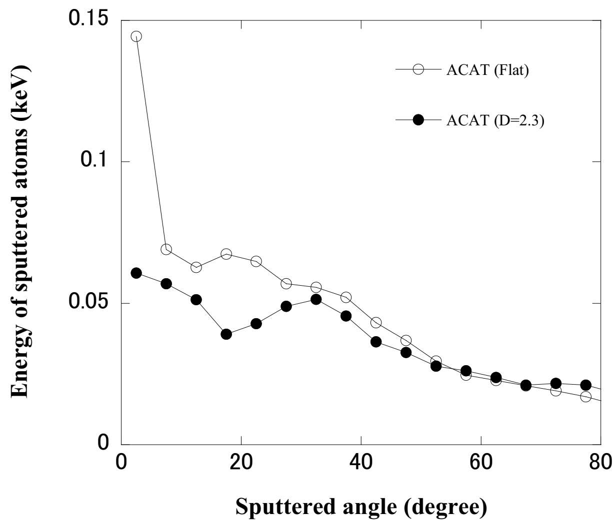

Fig. 7 Energies of sputtered atoms calculated by ACAT under 1 keV H^+ ions bombardment at an incident angle 80 degree from surface normal.

4. Conclusion

The angle and energy distribution of reflected particles are measured for pyrolytic graphite (HOPG) bombarded by 1 keV H^+ ions at an incident angle 80 degree from surface normal. The surface structure of HOPG observed by a SEM is bumpy.

In order to estimate the influence of the surface structure of the target material for reflection and sputtering, the fractal surface geometry have been employed into the ACAT code. From the ACAT calculations, the rough surface tends to suppress the peak angle dependence on reflection and sputtering due to the local incident angles. Although the difference between the experimental data and the fractal ACAT still remains, the ACAT results with the fractal model predict the tendency of the experimental data. The fractal surface model is a valid tool to estimate the rough surface.

Acknowledgements

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