Effects of Accumulation of Impurities in Target Materials for Sputtering

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1 Introduction

Sputtering yields have been measured for many ion-target combinations so far [1][2]. Monte Carlo simulation codes [3][4] have been developed to estimate ion-solid interactions, and are in good agreement with experimental data on sputtering yields [1][2]. Several empirical formulae which predict the energy dependence of sputtering yields for any ion-target combinations were proposed [2][5]. The Yamamura-Tawara semi-empirical formula [2], hereafter we abbreviate to Y-T formula, are applied to estimate sputtering yields in the present work.

Experimental works on the sputtering yields of carbon due to xenon ions have shown significant yields below the threshold energy predicted by the empirical formula at normal incidence [6-12]. The predicted threshold energy is 160.84 eV for the xenon–carbon combination in the Y-T formula [2]. In this paper we report the results of sputtering yields of carbon under the xenon ion bombardment calculated with a Monte Carlo code ACAT [4] to find the reason to explain the discrepancy between the experimental results and the predictions from the Y-T formula. Atoms of Xe are retained in graphite to make atomic xenon fraction as high as 14% after the low energy Xe plasma sputtering experiment [10]. We will correlate the amount of the incident particles retained into a target material and the resultant sputtering yields from graphite materials, under a continuous bombardment of Xe ions.

2 Calculation model

2.1 Monte Carlo simulation code ACAT

A Monte Carlo simulation code ACAT has been used to calculate sputtering yields of carbon from xenon containing carbon materials due to xenon bombardment in the present work. Since the ACAT code has been described in detail elsewhere [9], the main features of the code are briefly outlined here. The code numerically calculates trajectories of atoms colliding in an amorphous target based on the binary collisions approximation with the target atom positions assigned by a Monte Carlo method. The target atoms are thus, randomly distributed in each unit cubic cell, the lattice constant of which is calculated from $R_0 = N^{-1/3}$, where N is the atom number density of the target material. Target and retained atoms are assigned in each unit cell in accordance with the atomic fractions. The target and retained atoms are distributed uniformly over the target material. The lattice constant of the target material is determined from the density composed of target and retained atoms.

2.2 Threshold energy for sputtering

The threshold energy of sputtering, E_{th}, in the Y-T formula are given by

$$\frac{E_{th}}{U_S} = \frac{6.7}{\gamma}, \qquad M_1 \geq M_2, \qquad (1)$$

$$\frac{E_{th}}{U_S} = \frac{1 + 5.7(M_1/M_2)}{\gamma}, \qquad M_1 \leq M_2, \qquad (2)$$

where M_1 and M_2 are the masses of the projectile and the target atom, respectively. U_s is the surface binding energy of the target material. We take the heat of sublimation as the surface binding energy of the target material. The surface binding energy for carbon targets is 7.37 eV. γ is the energy transfer factor in an elastic collision.

3 Results

3.1 Effect of accumulation of Xe for carbon sputtering

Shown in Fig.1 are the sputtering yields of carbon in pure graphite bombarded by xenon ions calculated with ACAT together with the experimental data and the curve obtained from Y-T formula. The yields from ACAT agree well with the Y-T formula, but the ACAT results differ from the experimental data. The sputtering yields of carbon have been confirmed present even below the threshold energy predicted by eq. (1), which is 160.84 eV. The threshold energy obtained from ACAT result is similar to the threshold energy predicted by eq. (1), and is substantially larger than that obtained by experiments. Considering the present case where the mass of the projectile is larger than that of the target atom, no mechanism to reduce the threshold energy is predicted from the collision theory for pure carbon target [13]. The dominant process of sputtering in the case of $M_1 > M_2$ (Mechanism I) is shown in Fig. 2 (a) in the collision theory [13].

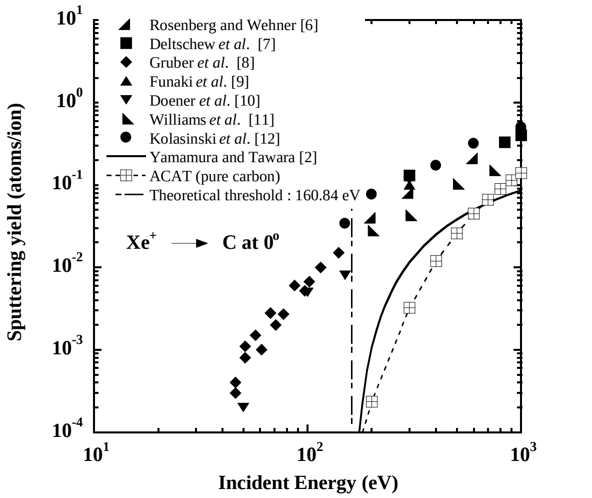
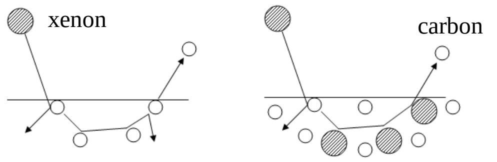


Fig.1 Experimental sputtering yields of carbon bombarded by xenon ions. Also shown in the figure are the results calculated with the Y-H formula and ACAT.

Figure 3 shows the results of ACAT with 14% xenon atoms retained in graphite together with the experimental data. The ACAT results are in good agreement with the experiments. The reason why the Y-T formula differs from the experimental data is that the model does not take into account the effect of accumulation of xenon in graphite. Considering the sputtering of carbon from graphite containing 14% xenon atoms, atomic collisions in the target consists of collisions between carbon-carbon, carbon-xenon and xenon-xenon. The threshold energy of sputtered atoms is determined by the process of minimum energy loss in the target material. In the xenon retaining system, the primary recoil carbon atoms produced by the incoming xenon ions can be sputtered out through the collisions with only xenon atoms in the target (Mechanism II in Fig. 2 (b)). Thus, the accumulation of xenon in graphite may lead to the reduction of the threshold energy for sputtering of carbon due to the xenon ion bombardment. Considering the projectiles are carbon and the target atoms are xenon, the threshold energy calculated by eq. (2) is only 36.5 eV, and this threshold energy is in good agreement with the experimental results.



(a) Mechanism I (b) Mechanism II

Fig. 2 Schematic representations of mechanism I and II. (a) pure carbon model. (b) recoil carbon collision with retained Xe atoms.

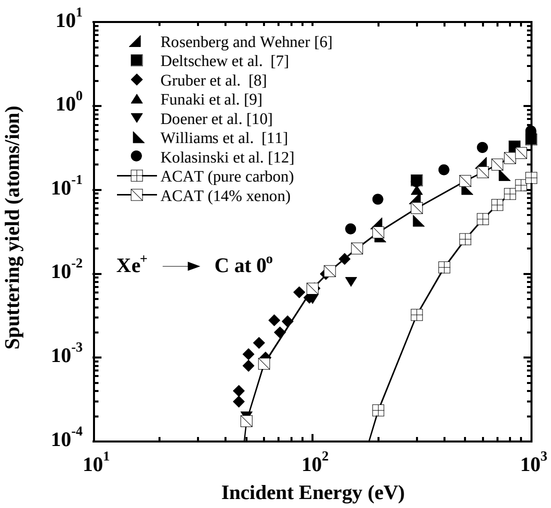


Fig.3 Experimental sputtering yields of carbon bombarded by xenon ions. Also Shown in the figure are the results calculated with ACAT with pure carbon and ACAT with graphite contained 14% xenon atoms.

4 Conclusion

The sputtering yields of carbon have been measured during xenon ion bombardment under the threshold energy predicted by the Y-T formula at normal incidence. We have confirmed the presence of the sputtering yields of carbon below the threshold energy by calculating the collision cascade in the xenon retaining carbon target with a Monte Carlo code ACAT. The yields of carbon calculated with ACAT are in good agreement with the experimental data. In other word, the retained xenon atoms in graphite enhance the sputtering yield of carbon below the threshold energy. This reduction in the threshold energy can take place in the case where the mass of the projectile is larger compared with that of the target atom.

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