§15. Simulation Study on Sputtering from Compound Materials at Elevated Temperature

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We have simulated surface compositional change in Hirooka's experimant[1] under 250 eV D^+ ion bombardment at high temperature. We applied ACAT-DIFFUSE code to calculation of compositional change of boronized graphite. The ACAT-DIFFUSE is a simulation code based on a Monte Calro method with a binary collision approximation and solves diffusion equations. The ACAT-DIFFUSE were developed to estimate chemical reaction such a methane production.

We adopted 2.5×10^{17} ions/cm^2/sec as a D^+ current density and the target temperature was set to be 550 °C. Ion bombarding energy is 250 eV. Target of bulk-bronized graphite contain 20% B atoms. The simulations were performed under the same condition as Hirooka's experiment. In this work, we assumed that vacancy and range distributions do not change during one layer removal. In the case of high incident energy (250 eV), this assumption seems to be valid, because boronized graphite does not represent apparent composition change due to deuterium ion beam bombardment.

Fig.1 shows the fluence dependence of the change of B and C concentrations at the topmost layer. Here the two cases are calculated. One is the case under kinetic mechanism only. The other is the one case under both kinetic mechanism and chemical reaction. When boron carbide (or B_4C) are bombarded with ion beam, boron atom is sputtered preferentially due to difference of surface binding energy. However, boron does not show significant preferential sputtering with light ion bombardment at high energy. Therefore, in fig. 1 bulk-bronized graphite does not show apparent compositional change near the surface under light ion bombardment. However, Hirooka's experiment shows that boron is slowly enriched to ~30% as the fluence approaches the order of 10^{21} D^+ions/cm^2 at 550°C. It seems that this enrichment is attribute to the preferential chemical sputtering of boron. At 550°C, methane formation is only take into account. Methane formation is estimate by eq. (1).

$$\frac{dn_D}{dt} = J_D^s - 4K_1K_2k_3 \cdot n_D^3 + D\left(\frac{\partial n_D}{\partial x}\right)_{x=0} \qquad (1)$$

Here J_D^s is surface concentration of deuterium due to D^+ ion bombardment. The first term on the right hand side of eq. (1) represents the rate of adsorption of D^+ ions per unit surface area from the primary beam. The third term represents methane production. The last term on the right hand side of Eq. (1) represents diffusion into and out of the bulk solid. Methane reaction rate are estimated by following equation:

$$K_1K_2k_3 = A_1 \exp(-E_{CH_4} / k_BT) \qquad (2)$$

Here A_1 is constant. E_{CH4} is activation energy of methane production. k_B is Bolztmann constant.

The calculated result inclueding chemical reaction shows that boron is enriched to ~23% as the fluence approaches the order of 10^{21} D^+ions/cm^2. In present work, we obtained the result which has about 20% difference between experimental data and the ACAT-DIFFUSE data. More detail study is required to explain this difference.

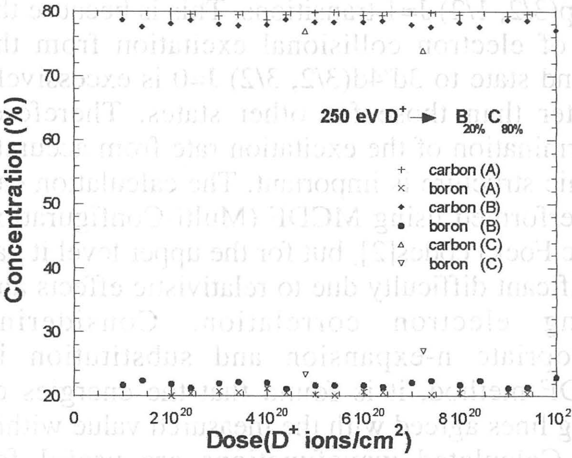

Fig. 1 The fluence dependence of the change of B and C concentrations on boronized graphite surface

Here, A means the calculation including kinetic mechanism only. B means the calculation including *both* kinetic mechaniam and methane formation. C means Hirooka's experimant.

[1] Y. Hirooka et al, Fusion Tecnol. 19(1991)205