§28. Study on Tungsten Nano-structure Formation

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1. Introduction

Under helium plasma irradiation, "bubble" structure is formed around the surface of tungsten[1,2]. For the special case in which tungsten temperature is 1000-2000 K and incident energy of helium plasma is 20-100 eV, nanofilament structure, called "fuzz" structure, is generated on the tungsten surface [3,4]. To explain these experimental results, theories [5-7] of the formation of the fuzz structure have been proposed. We reproduced[6,7] the fuzz structure by hybrid simulation combining between molecular dynamics and Monte-Carlo methods.

2. Simulation methods and results

In the simulation for Ar irradiation to tungsten target, we calculated the three physical quantities, that is, sputtering yield *Y*, range *R*, and retention rate *A*.

The sputtering yield Y is obtained as follows. In $N_{\text{sim}} = 200,000$ simulations for the tungsten target with N = 10, 20, 30, 40, and 50 half-spheroid holes with polar radius d and equatorial radius $r = 5\text{\AA}$; the number of tungsten atoms released from the tungsten surface were counted as N^{sp}_{W} . The sputtering yield Y is given as $Y = N^{\text{sp}}_{\text{W}}/N_{\text{sim}}$.

We investigate the dependence of the thickness of the fauzz structure. It is expected that the polar radius of the half-spheroid-hole *d* corresponds to the thickness of the fuzz structure. We, therefore, changed the aspect ratio as d=r=0, 1, 3, 5, 7, 10, 30, 50, 70, and 100, where r=5Å, and the number of holes is fixed to 50. Figure 2 shows that as the d = r becomes larger the *Y* decreases and converges on $Y \sim 0.025$, which is 28 % of the $Y(d=r=0) \sim 0.087$.

3. Conclusion

Using BCA simulation code AC \forall T, we calculated



Fig. 1. The initial condition of the tungsten target. N=10, 20, 30, 40, and 50 half-spheroids are hollowed from a flat BCC tungsten surface (100). (a)The equatorial radius r of the half-spheroids is set to 5Å, and the polar radius d is chosen among 5, 50, and 1000 Å. (b) An argon atom with 100 eV is injected into this tungsten target. The o-xyz coordinate is used in the simulation.



Fig. 2. Sputtering yield *Y* vs. the aspect ratio d = r = 1, 10, and 100, where r = 5Å in the case that the number of half-spheroid holes is 50.

the sputtering yield, the range, and the retention rate for the tungsten with the rough surface under the argon atom irradiation. We found from the simulation that the sputtering yield decreases and the retention rate increases, as the surface becomes rougher. From this result that these quantities depend on the surface strongly, we suggest that it is necessary to consider the surface structure of the tungsten target in estimating the effect from the wall.

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