J. Plasma Fusion Res. SERIES, Vol. 3 (2000) 288–292

Time Evolution of Surface Topography of Plasma Facing Materials with Non-Uniform Impurity Deposition

OHYA Kaoru*, KAWAKAMI Retsuo and AIZAWA Hiroshi
Faculty of Engineering, The University of Tokushima, Tokushima 770-8506, Japan

(Received: 18 January 2000 / Accepted: 6 June 2000)

Abstract

The development of the surface topography and its influence on the erosion rate of plasma facing materials are simulated. The calculations start with slight irregularities (10 nm range) of the surface and change with time due to the dependence of the sputtering yield on ion and target species as well as on the angle of incidence. The topography of a boron surface with an initial non-uniform carbon deposition drastically changes due to high-fluence deuterium ion irradiation. Sharp triangular cone like structures develop at the beginning of the irradiation. The calculations simulate the experimental observation in TEXTOR-94 where the initial slow erosion of a boron film was followed by an accelerated erosion and the eventual decrease of the rate. Deposition of implanted carbon occurs more at the grooves between cones than the top. This tends to fill the grooves.

Keywords:

plasma facing component, surface topography, boron erosion, carbon deposition, computer simulation, simultaneous erosion/deposition

1. Introduction

For long-pulse or steady-state operation of magnetic fusion devices, sputter erosion leads to a shortened lifetime of plasma facing components (PFC). Deposition of impurities, which are eroded at the other locations and transported in a plasma, may reduce the net erosion rate of the PFCs, but the erosion/deposition will also modify the surface morphology, which alters the lifetime of the PFCs. Recently, the erosion of a thin boron film (a-B:D) of ~100 nm on a graphite block under simultaneous carbon deposition has been observed in TEXTOR-94 [1]. The erosion rate was not constant with time at a fixed location; the initial thickness began to changes with accelerating erosion rates and eventually with dropping rates. Furthermore, the non-uniform carbon deposition, in the range of 10–30 μm, on a boron film was discovered in another experiment [2].

In this study, the development of the surface topography is simulated with the initial condition of a slight non-uniform carbon deposition on boron. The aim of this paper is to discuss the changes in surface topography and its influence on the erosion rate, due to measured ion fluxes of deuterium (D) and carbon (C) impurity.

2. Model for Surface Topography Development

A two-dimensional sinusoidal change in thickness of carbon deposition of $y = a\sin(x/b)$ on a flat boron surface ($y = -a$) is assumed and the surface is bombarded in the negative y-direction by an ion flux, Γ, as shown in Fig. 1. The incremental value, Δy, of displacement of y-value at constant x on the surface during the lapse of the time Δt, is evaluated to be (Γ/

*Corresponding author's e-mail: ohya@ee.tokushima-u.ac.jp

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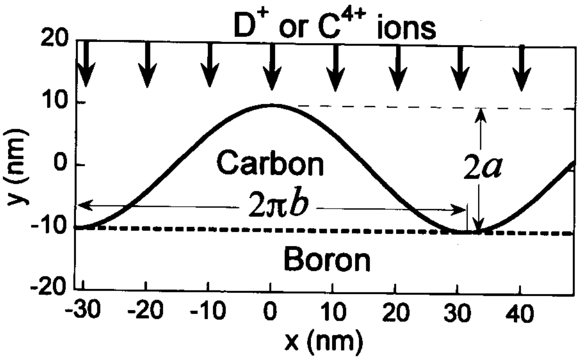

Fig. 1 Two-dimensional model for surface topography of boron with sinusoidal deposition of carbon: $y = a\sin(x/b)$, $a = b = 10$ nm.

$N)Y(E_i,\theta)\Delta t$, and the new y-value is obtained by subtracting the value from the original one. Here, N is the atomic density of the target and $Y(E_i, \theta)$ the sputtering yield as functions of incident ion energy, E_i, and the angle of incidence, θ, with respect to the normal. The angle θ is simply evaluated from the slope of the surface by taking sampling points along x-axis. To avoid non-correctable computer errors due to finite Δt and Δx (the interval of sampling points), the present simulation takes into account two correction procedures as presented by Ishitani *et al.* [3]. One is a removal of any overestimate of Δy, which reverses the slope of the surface, with Δt. Another correction is an averaging technique in the calculation of Δy, so that $(\Delta y_{n-1} + 2\Delta y_n + \Delta y_{n+1})/4$ is used instead of Δy_n at the nth sampling point. These corrections are based upon the practical situation that the sputtering process is dictated by a collision cascade of finite dimensions, so that it is unrealistic to consider that the apical point can remain to be unaffected by neighboring sputtering. As a result, the motion of an initially $\theta = 0$ point is also dictated by neighboring points.

The angular dependence of the sputtering yield is described according to Yamamura *et al.* [4] by $Y(E_i, \theta) = Y(E_i,0)(\cos\theta)^{-f}\exp\{f[1 - (\cos\theta)^{-1}]\sin\eta\}$ with fitting parameters f and η. For the impact of D ions $f = 2.24$ and 2.53 for boron and carbon, respectively, whereas $\eta = 0.161$ rad and 0.151 rad. For normal incidence, the sputtering yield $Y(E_i,0)$ is calculated by using the Bohdansky formula [5]. For simplicity, instead of experimentally observed a-B:D (1×10^{23} B/cm^3) and a-C/B:D (0.65×10^{23} C/cm^3) films, a boron with an infinite thickness and the density of crystalline boron (1.3×10^{23} B/cm^3) under a very small size of deposition of pure carbon (1.1×10^{23} C/cm^3) with $a = b = 10$ nm is assumed to be exposed to the edge plasma in TEXTOR-94. In the experiment [1], the boron surface (6 cm $\times$ 6.3 cm) was declined by 20.8° to the toroidal magnetic field, so that the different locations in the boron surface corresponded to different radial distances from the last closed flux surface (LCFS: $r = 46$ cm), which ranged from 47.2 cm to 49.5 cm. The total exposure time of 121 s during 22 discharges was shared to an ohmic heated (OH) phase of 95 s and an auxiliary heated phase of 26 s (neutral beam injection, NBI). In the simulation, the electron temperature, T_e, and the ion fluxes, Γ_D and Γ_C, at the boron surface are average values weighted by the exposure times in the OH and NBI phases; $T_i = T_e$ is assumed, where T_i is the ion temperature. The energy of the ion bombarding the surface, E_i, is approximately the sum of the thermal energy and the acceleration due to the sheath potential: $E_i = 2T_i + 3QT_e$, where Q is the charge state of the ion [6]. The values of E_i, Γ_D and Γ_C decrease exponentially with increasing radial distance, r. At each point of the surface from $r = 47.3$ cm to $r = 49.1$ cm, E_i for D^+ (C^{4+}) ions ranges from 76 eV (213 eV) to 31 eV (86 eV), whereas $\Gamma_D{}^+$ ($\Gamma_C{}^{4+}$) from 1.0×10^{18} cm^{-2}s^{-1} (8.4×10^{15} cm^{-2}s^{-1}) to 2.0×10^{17} cm^{-2}s^{-1} (3.4×10^{15} cm^{-2}s^{-1}).

3. Results of Calculation

The physical sputtering yield of boron due to the impact of D ions increases with the angle of incidence θ, reaches a maximum of about 2 to 3 times larger than the value for normal incidence ($\theta = 0$) at about $\theta = 70°$ and returns to an apparent zero at $\theta = 85° \sim 90°$. Points between the extreme y values on the sinusoidal curve of the surface, therefore, are more eroded than near the maximum and minimum points of the curve. Even if carbon is not deposited (Fig. 2(a)), the maximum of the curve becomes sharp in the early stage of exposure; but with further exposure the resulting wave-like structure shrinks gradually. This development of the surface profile results in slight non-linear change in the erosion rate at the maximum point of the profile in the early stage (Fig. 2(b)). The rate decreases with increasing radial distance, due to the decrease of both the ion temperature and the ion flux.

If an initial condition of a sinusoidal carbon deposition is assumed on the boron surface, the film behavior drastically changes not only the development of the surface profile but also the erosion rate. This is shown in Fig. 3. At the energies of less than 1 keV, the sputtering yield of carbon is smaller than the yield of boron, therefore, the surface location where thick carbon

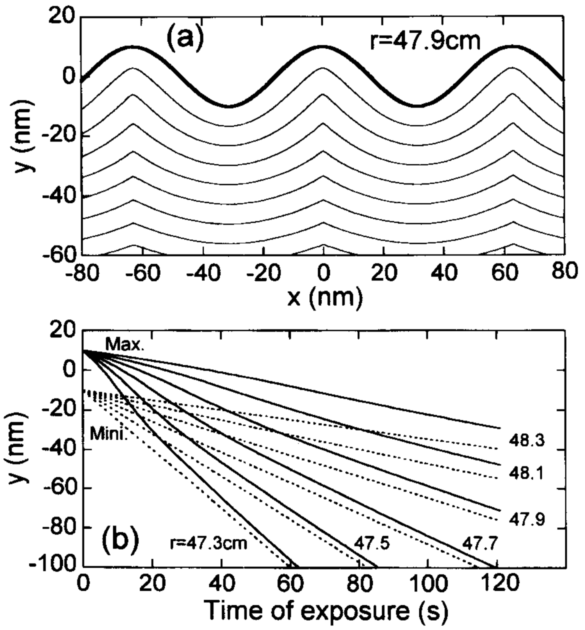

Fig. 2 (a) Development of sinusoidal surface of boron at the radial distance of $r = 47.9$ cm from the plasma center at 6 s intervals under D^+ ion sputtering. (b) Time evolution of its erosion at the maximum and minimum points of the surface at different radial distances.

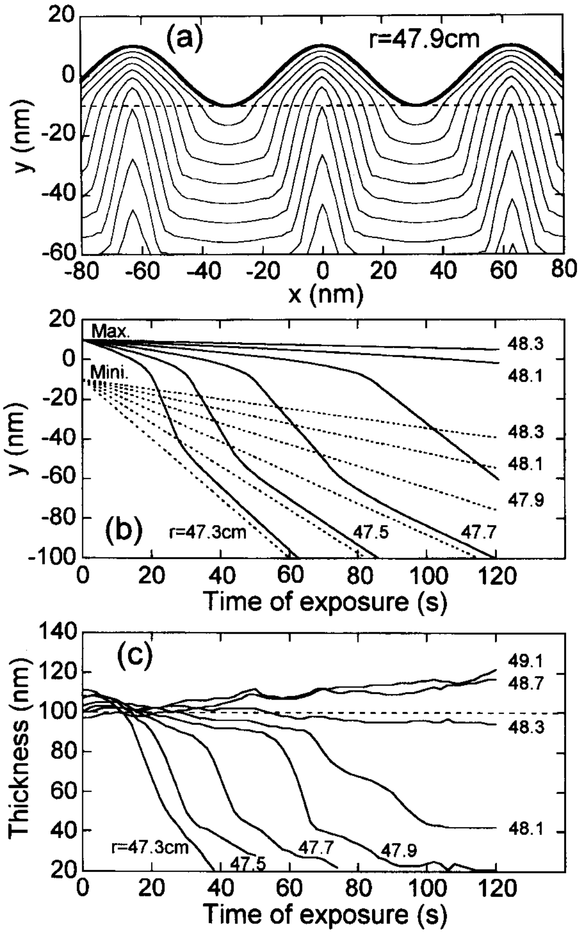

Fig. 3 (a) Development of a boron surface with an initial condition of a sinusoidal carbon deposit at the radial distance of $r = 47.9$ cm from the plasma center at 6 s intervals under D^+ ion sputtering. (b) Time evolution of its erosion at the maximum and minimum points of the surface at different radial distances. (c) Observed changes in the thickness of boron film at different radial distances in TEXTOR-94 [1].

deposition occurs is less eroded, whereas the carbon-free areas are more eroded. The non-uniform erosion enhances the initial surface imperfections, like as cones, at the early stage (Fig. 3(a)). As far as new carbons are not deposited, with further exposure, the cones shrink in the same way as the wave-like profile in Fig. 2(a). Although the carbon deposition suppresses the erosion rate of boron at the early stage of exposure, the enhancement of the surface imperfections accelerates the rate at the side areas of the cones due to increased angles of bombarding ions. As shown in Fig. 3(b) the initially reduced erosion is followed by a steep increase in the rate, which is two or more times larger than that for the initially deposited carbon. The erosion lasts until the rate is reduced to that at the minimum point of the surface structure. These erosion features of boron with a non-uniform carbon coverage are very similar to the time evolution of a boron (a-B:D) film exposed in an edge plasma of TEXTOR-94 (Fig. 3(c)).

The morphological change and erosion of carbon-deposited boron are little influenced by the impact of C impurity ions out of the plasma (Fig. 4). This is due to their small fraction (0.84–1.7%) of total ion flux to the surface and the much less dependent sputtering yields for boron and carbon on the angle of incidence ($\theta < 60°$), in spite of an about 10 times larger sputter yield for C^{4+} ions compared to D^+ ions. The reflection coefficient of C ions from carbon and boron is very small for normal incidence, but increases largely with oblique incidence. This may cause that the implanted C ions, which are not reflected, are deposited non-uniformly on the sinusoidal surface. The morphological change of the surface is calculated in Fig. 5(a), and tends to fill the valleys. The deposition of implanted carbons can explain the experimentally observed net deposition of carbon at large radial distances ($r > 48.7$

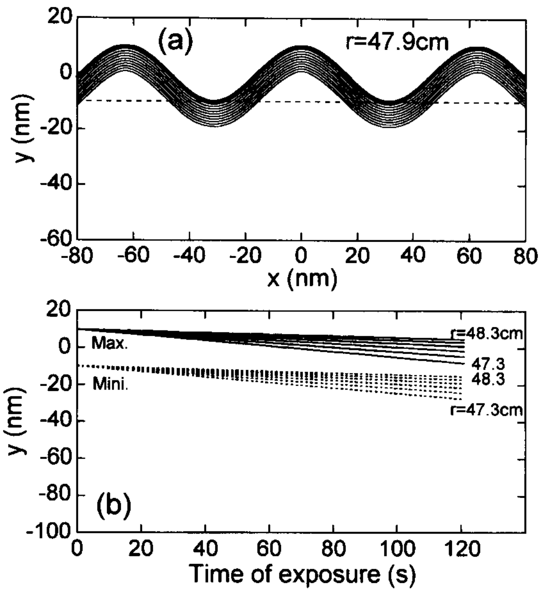

Fig. 4 (a) Development of a boron surface with an initial condition of a sinusoidal carbon deposit at the radial distance of r = 47.9 cm from the plasma center at 6 s intervals under C^{4+} ion sputtering. (b) Time evolution of its erosion at the maximum and minimum points of the surface at different radial distances.

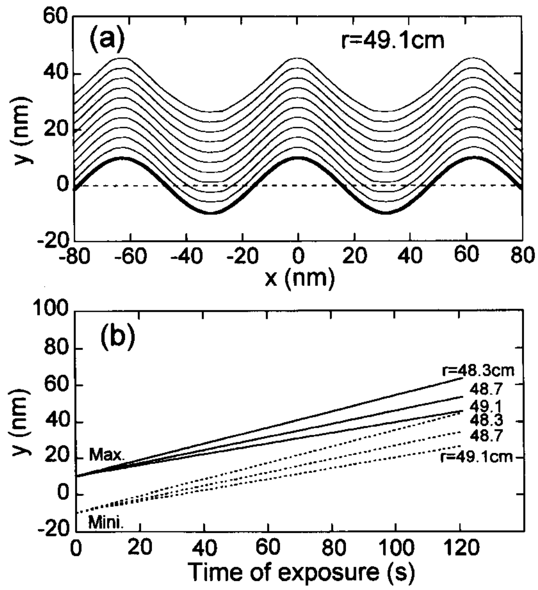

Fig. 5 (a) Development of a boron surface with an initial condition of a sinusoidal carbon deposit at the radial distance of r = 49.1 cm from the plasma center at 6 s intervals under C deposition. (b) Time evolution of its deposition at the maximum and minimum points of the surface at different radial distances.

cm) in Fig. 3(c), whereas the increasing thickness at small distance (r < 48.3 cm) cancels the sputter erosion due to the impact of D ions (Fig. 3(b)).

4. Discussion

The dynamic change of composition due to the implantation of carbon impurities in the surface layer causes a strong decrease in the boron sputtering yield and a formation of the carbon-boron mixed layer. This can explain the experimental observations of a lowering of the surface erosion at the early stage of the plasma exposure near the LCFS and a carbon deposition at the surface location far from it. However, the non-linear erosion rates, discussed here, were not reproduced by the previous TRIDYN dynamic simulation [7].

The simulation calculation are based on an assumption of sinusoidal carbon coverage with the range of 10 nm on a boron film, which is clearly different from the experimentally observed ranges (10–30 μm) [2]. Nevertheless, plasma-irradiated surfaces will feature an atomic-scale imperfection with the macroscopic structure superimposed. Furthermore, the assumed initial condition leads to an simulation of the observed change of the erosion rate with time, therefore, the validity of our model can not be excluded. Although the physical sputtering yield of boron due to the impacts of D ions is larger than that of carbon, the observed erosion rate of a-B:H films in hydrogen plasma is in general smaller than that of a-C/B:H films [8]. This indicates the dominance of chemical erosion of carbon in a-C/B:H films. The use of the experimental sputter yield of the hydrogenate films had led to an explanation of the experimental results by using time-dependent C concentration of the boron film [1].

The cones produced by non-uniform carbon deposition on the boron surface are unstable, i.e., they develop but finally shrink after long-time irradiation with D ions, due to the correction procedures for the calculation mentioned above. If the angle of incidence will be set to zero for the maximum and minimum points of the sinusoidal surface (Fig. 1), the cones never disappear as calculated for an molybdenum-seeded spot on copper by Hirooka *et al.* [9]. However, it is not clear for real surfaces whether individual cones survive or new cones appear to replace disappearing cones during continuous carbon deposition.

If the deposited impurities are sufficiently mobile, they tend to agglomerate [10]. The surface mobility and carbon agglomeration is perhaps one process to form growing islands on the surface, although the agglomerates in the range of 10–30 nm were not observed after long-time irradiation. A second possibility for carbon transport across the surface might be the emission and direct transport in the edge plasma, followed by the re-deposition.

5. Conclusions

Surface topography of a boron surface with non-uniform carbon deposition drastically changes due to high-fluence D ion irradiation. A sharp triangular structure like as a cone is developed at the early stage. As long as new carbons are not deposited, however, it finally shrinks after long-time irradiation. The calculations reproduce the experimental observation in TEXTOR-94 that the initial slow decreases of boron were followed by large drop and the eventual decrease in the erosion rate. Erosion by C ion impact causes much less change of the topography, whereas the deposition of implanted carbon occurs more in the grooves between cones than the top.

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