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Journal of Nuclear Materials 329–333 (2004) 732–736
journal of nuclear materials
www.elsevier.com/locate/jnucmat

Modeling of erosion and deposition patterns on C–W and W–Ta twin limiters exposed to the TEXTOR edge plasmas

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Abstract

The erosion and deposition patterns on tungsten and tantalum test limiters exposed to the TEXTOR deuterium plasma containing a small amount of C impurity are simulated with the modified EDDY code. At the very top of the W and Ta limiters, there occurs neither erosion nor deposition, but the erosion proceeds slowly along the surface. When approaching the edge, the surface is covered by a thick C layer, which shows a very sharp boundary similar to the observation in surface measurements. In the erosion zone, the re-deposited carbon forms a W (Ta)–C mixed layer with small C concentration. Assumptions for chemical erosion yields of $\sim$0.01 for W and $<$0.005 for Ta fit the calculated widths of the deposition zone to the experimentally determined values. Possible reasons for the difference between W and Ta are discussed.

1. Introduction

High-*Z* metals of high melting point are extensively studied as candidate materials for plasma-facing components for the next-step fusion device, e.g., ITER. Besides erosion of tungsten (W), post-mortem analyses of a W test limiter [1] and divertor tiles [2] showed a pronounced deposition of background plasma carbon (C) impurity. The deposited C also contained a considerable amount of hydrogen isotopes. In recent twin test limiter experiments in TEXTOR [3], erosion zone was clearly separated from C deposition zone that appeared at the edge of the W part of the C–W twin test limiter, as well as for the W limiter, after the plasma exposure. On the tungsten–tantalum (W–Ta) twin test limiter [4], the extent of the deposition area was distinctly broader on Ta than on W exposed to the plasma under the same condition.

In previous studies [5], the erosion and deposition processes of W under simultaneous bombardment with deuterium (D) ions and a small amount of C ions were investigated by using a dynamic plasma-surface interaction code, EDDY. We showed that the transition from the deposition to the erosion abruptly occurred when the plasma temperature was increased. In this paper, the erosion and deposition patterns on the W and Ta limiters are simulated by the modified EDDY code. We concentrate our attention on the observed difference between the W and Ta parts of the W–Ta twin test

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doi:10.1016/j.jnucmat.2004.04.183

limiter. Many physical properties of both metals are similar, but there are differences in thermal conductivity and affinity for hydrogen, i.e., trapping efficiency. The differences caused the surface temperature during plasma exposure to be higher for Ta than for W, and the amount of D retained was two orders of magnitude larger in Ta than in W [6]. The influence of chemical erosion, i.e., hydrocarbon formation, and thermal diffusion of the deposited C on W and Ta at elevated temperatures are also discussed in the paper.

2. Simulation models for erosion and deposition patterns on W, Ta and C limiters

The EDDY code models the interaction of plasma ions, e.g., D^+ and C^{4+} ions with surfaces. Maxwellian distributions of ion velocities are taken into account and ions are accelerated towards the surface by the sheath potential, V_{sh} defined as $V_{sh} = (T_e/2)\ln(\pi m_e/m_i)$, where T_e is the electron temperature. Equal temperatures of electrons and ions, $T_e = T_i$ are assumed. The code simulates slowing down of projectile ions in the solid and the formation of recoil cascades leading to processes such as ion reflection and physical sputtering. Dynamic changes in the composition of the irradiated material arise from deposition of C ions, collisional transport of the deposited C atoms, and, at elevated temperatures, thermal diffusion into the material. The surface segregation and phase formation, e.g., formation of WC and W_2C, are not taken into account. Chemical sputtering of the deposited C by the impact of D ions is included, where constant erosion yields of 0.005–0.04 are assumed. The detailed description of the EDDY code has been presented previously [5].

The EDDY code has been modified to simulate the erosion and deposition patterns on test limiters exposed to edge plasma at the TEXTOR tokamak. The test limiter is 12 cm long in toroidal direction and 8 cm wide in poloidal direction with a spherical shape (radius of 7 cm). It consists of two parts: one half made of W and the other half of Ta or C. In the simulation calculations, each half of the spherical area, W, Ta or C, is divided into $N_{polar} \times N_{azimuth}$ segments in both polar and azimuthal directions. In this study, $N_{polar} = 10$ and $N_{azimuth} = 18$, where the polar angle ranges from 60° (edge of the limiter) and 0° (top of the limiter), and the azimuthal angle ranges from 0° to 180°. In each segment, the dynamic erosion and deposition processes are simulated using the code. Sputtered and reflected impurities undergo successive ionizations and dissociations by plasma electrons and ions. Some of those impurities are promptly re-deposited on the same segment where they were released, or re-deposited on the other segment after migration in the plasma [7]. In this study, such re-deposition processes are not taken into calculation. In the experiments, the top (the tangency point) of the limiter was positioned at the radial distances, r, of 46.5–47.5 cm from the plasma centre. The plasma radius was defined by the position of the main toroidal belt limiter, $r = 46$ cm. Due to the spherical shape of the limiter, the limiter edge was ~3.5 cm from the top in the radial direction and each point on the surface corresponds to a different radial distance. Assuming symmetry in the toroidal direction, radial profiles of the plasma electron density, n_e and temperature measured by a He atomic beam are fitted to an exponential function as input parameters for the modified EDDY code. Each discharge corresponds to different n_e and T_e profiles, but typically they are represented by $n_e = 6.3 \times 10^{12}$ cm^{-3} and $T_e = 58$ eV at $r = 46$ cm. n_e and T_e decrease with increasing radial distance with a decay length: $\lambda_{ne} = 3.2$ and $\lambda_{Te} = 2.5$ cm, respectively. The bombarding ion fluxes calculated from the values of n_e and T_e are reduced due to the inclination angle of each point on the surface to the lines of the toroidal magnetic field (2.25 T). The maximum ion flux ($\sim 1.5 \times 10^{19}$ cm^{-2} s^{-1}) appears at the toroidal position of ~3.0 cm from the top of the limiter. When approaching the plasma edge, the C concentration in the plasma is increased to change from 2% (in the C/(D + C) ratio) at the top of the limiter to 5% at the edge.

3. Results and discussion

Since each point on the spherical surface of the limiter corresponded to a different radial distance from the plasma centre, the erosion or deposition thickness depends on the position on the surface. As shown in Fig. 1, at the very top of the limiter (at the tangency point: $d \sim 0$), there occurs neither erosion nor deposition due to the grazing incidence of the ions on the surface. But the erosion proceeds gradually as the bombarding ion flux increases along the surface. When approaching the limiter edge, the surface is dominated by strong C deposition, which results in the formation of a thick layer of the deposited C on W and Ta. A comparison of the calculated thickness with the observed areal C density in surface measurements results in a density of $\sim 3 \times 10^{22}$ cm^{-3} for the deposited C, which indicates a non-uniform C deposition on W since the present calculation assumes the density of 1×10^{23} cm^{-3}. The transition from erosion to deposition shows a very sharp boundary, similar to the observed patterns on the W limiter [3]. When the limiter is retracted to larger radial distance from the plasma centre, the deposition area broadens towards the top of the limiter. Thus, under the exposure at $r = 49$ cm no erosion occurs over the whole area.

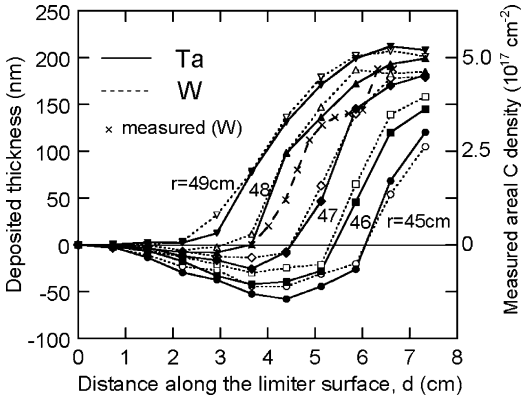

Fig. 1. Deposited thicknesses along the surfaces of the Ta and W limiters. The limiters are positioned at radial distance, r, from 45 to 49 cm, and the total fluence of the bombarding D ions, including small amount of C ions, is 1×10^{22} cm^{-2}. The distance along the limiter surface is measured from the top ($d = 0$ cm) to the edge ($d = 7.3$ cm). The chemical sputtering is not taken into calculation. Positive values in the ordinate represent net deposition and negative values represent net erosion. Experimentally determined carbon concentrations on the W part of the C–W twin limiter are taken from [3].

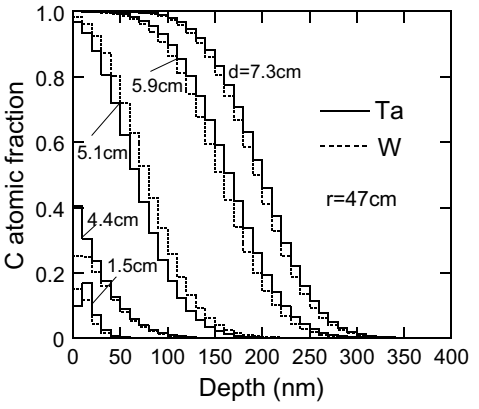

Fig. 2. Depth profiles of C at different distances along the surfaces of the Ta and W limiters. The limiters are positioned at $r = 47$ cm. The chemical sputtering is not taken into account in the calculation.

The difference between W and Ta appears in the extent of the erosion zone where the erosion thickness is slightly larger for Ta than for W, due to the different surface binding energies, U, for Ta ($U = 8.10$ eV) and W ($U = 8.68$ eV). Atomic masses are very similar for both elements. Under the bombardment by low-energy light ions (<several hundreds of eV), due to small energy transfer from the ions to recoil atoms, the sputtering yield is largely influenced by U, and it is dominated by the threshold effect for physical sputtering. On the other hand, any noticeable difference between W and Ta is not found in the deposition zone where a thick C layer appears. The calculated depth profiles of the deposited C in the bulk (W or Ta) show characteristic changes when the transition from the deposition to the erosion occurs, as shown in Fig. 2. After the transition, there is no thick C layer and the deposited C is mixed with the bulk material, where the C concentration is substantially decreased. On the surface of the W (or Ta)–C mixed layer, the amount of incoming C ions (from the plasma) balances that of released C atoms (by C reflection and C sputtering) [5]. Therefore, a steady state condition is reached, where the limiter surface is eroded only by the bulk material sputtering with the reduced yield from the mixed material.

While in Figs. 1 and 2 chemical sputtering is not included, in further simulations constant sputtering yields, Y_{ch} of 0.005–0.04 are assumed for chemical sputtering. When a projectile D ion is implanted in the deposited C layer or the W (Ta)–C mixed layer, a hydrocarbon molecule (e.g., CD_4) is released with the emission probability related to Y_{ch}. If so, the areal density of C atoms in the layer is reduced by the bombarding D ion flux, and as a result, the surface is eroded; the implanted D with no chemical sputtering is assumed to be re-emitted immediately after the implantation. The inclusion of the chemical sputtering drastically changes the erosion and deposition patterns on the limiter surface for both W and Ta (Fig. 3) due to the corresponding change in the depth profiles of the deposited C. With increasing Y_{ch} the deposition areas tends to be more and more limited to the zone near the limiter edge, and at high Y_{ch} of 0.04, no deposition is calculated on the whole surface, where W (Ta)–C mixed layers are formed with very small C concentration. Therefore, the erosion

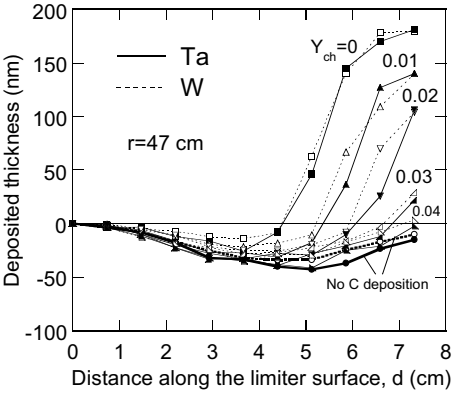

Fig. 3. Deposited thicknesses along the surfaces of the Ta and W limiters. The limiters are positioned at $r = 47$ cm. The chemical sputtering yield, Y_{ch} is assumed to be 0 (no sputtering), 0.01, 0.02, 0.03, 0.04. The thick solid and dotted lines represent the thicknesses on the Ta and W limiters, respectively, assuming no deposition of C.

thickness approaches the thickness of pure W (Ta) material (no C deposition). No difference between W and Ta is calculated if Y_{ch} is the same as for both. Since a recently observed Y_{ch} of tungsten carbides was much smaller than C materials [8], the mixed layer will be less influenced by chemical sputtering than for the deposited C.

The surface temperature measured during the exposure was higher for Ta (max. 2100 °C) than for W (max. 1600 °C) for identical discharges, mainly due to the difference in the thermal conductivity. The temperature distribution along the limiter surface was non-uniform [9]; the maximum temperature was measured far from the top along the limiter surface, e.g., $d \sim 2$ cm. Strong dependence of Y_{ch} on the temperature causes the C deposition thickness to reduce at the limiter edge but the W (Ta)-mixed layer is less influenced due to the higher temperature than a temperature (~800 K) where Y_{ch} is maximum. Furthermore, at the elevated temperatures, the deposited C appears to have diffused inside the bulk [10,11]. The diffusion coefficient of C in W is estimated by extrapolation of the observed values at 1030 and 1073 K by Schmid and Roth [11], e.g., 6.7×10^{-16}, 3.7×10^{-14} and 1.46×10^{-13} $cm^2\,s^{-1}$ for 1000, 1500 and 1800 K, respectively. The diffusion coefficient of C in Ta was observed to be three orders of magnitude smaller than in W around 1000 K (e.g., 9.5×10^{-20} $cm^2\,s^{-1}$ at 1000 K) by Rafaja et al. [12]. However, at increasing temperature, the diffusion coefficient increased much faster for Ta than the coefficients estimated here for W. Therefore, the diffusion coefficients at 1500 K are approximately similar for both metals and at 1800 K, the coefficient in tantalum is 5.1×10^{-11} $cm^2\,s^{-1}$, i.e., it is much larger than for tungsten. In this calculation, under typical exposure conditions for the W and Ta limiters (exposure time of 100 s) the erosion and deposition patterns on the limiters positioned at $r = 47$ cm are only slightly changed, except for Ta at 1800 K where the deposited C is strongly diffused into the bulk. This diffusion leads to the formation of a thick Ta–C mixed layer on Ta, instead of the thick carbon deposited layer. Furthermore, the erosion zone on the limiter surface disappears due to the retention of the deposited C moving inside the bulk [5].

Fig. 4(b) shows the calculated width of the deposition area on the W and Ta limiters as a function of radial distance from the top of the limiters. The deposition width is defined as the distance from the edge of the limiters to the position where the transition from the deposition to the erosion occurs, along the limiter surface. The deposition width increases with increasing radial distance and decreases with increasing chemical sputtering yield. As shown in Fig. 4(a), the observed widths were approximately 2 and 3 cm on the W and Ta limiters, respectively, positioned at 46.5–47.5 cm during accumulated plasma exposures of the order of 100 s. The comparison of the observation with the calculated

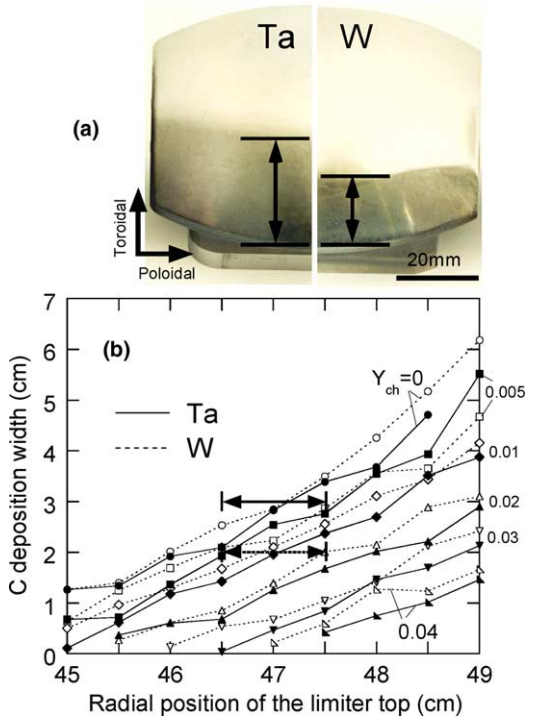

Fig. 4. (a) View of carbon deposits on the Ta and W parts of the W–Ta twin limiter [4]. (b) Calculated deposition widths along the Ta and W surfaces, including chemical sputtering with different yields ($Y_{ch} = 0$, 0.005, 0.01, 0.02, 0.03 and 0.04), as a function of radial position of the top of the limiters. The solid and dotted arrows represent the observed widths on the Ta and W surfaces, respectively, positioned from 46.5 to 47.5 cm.

widths dependent on the chemical sputtering yield allows for rough estimation of the chemical sputtering yields of the deposited C near the boundary between the erosion and deposition, both on W and Ta. As shown in Fig. 4(b), the estimated yield is ~0.01 for chemical sputtering of the deposited C on W, whereas the yield on Ta is much smaller than on W. The reduced yield for chemical sputtering of the deposited C on Ta can explain the reason that the extent of the observed deposition area is broader on Ta than on W. The yield for chemical sputtering of C test limiters exposed to the TEXTOR edge plasmas decreases from 0.04 to 0.01 for an increase in temperature from 800 to 1300 K [13]. Since the surface temperature was 10–30% higher for Ta than for W, the reduction of chemical sputtering of the deposited C on Ta at the elevated temperature may be one of the possible reasons for the broader deposition on Ta, in addition to the diffusion effect of the deposited C, as discussed above. The chemical sputtering yield (~0.01) of the deposited C, which forms the W–C mixed layer, is in good agreement with that observed for tungsten carbides [8]. However, the deposited C in the deposition

zone, which forms a thick C layer, may be strongly re-eroded due to an enhanced chemical sputtering yield (~0.1) [14,15].

Tungsten is an endothermic absorber of hydrogen isotopes, whereas Ta shows exothermic properties. After the plasma exposure, the amount of D retained in Ta was observed to be two orders of magnitude larger than in W, due to higher diffusion of D in Ta, especially at low temperature [6]. The diffusion of the retained D in the Ta bulk may limit the hydrocarbon formation, i.e., chemical sputtering, in the deposited C on Ta. This also causes the shift in position of the deposition-to-erosion boundary towards the top of the limiter as expected from Fig. 3. This will be another reason that the extent of the C deposition area is broader for Ta than for W. The total exposure time was twice as great for W (231 s) as for Ta (136 s); furthermore, each discharge corresponds to different plasma temperature and density. The different plasma parameters during the exposures are also an important reason to be taken into account in explaining the results.

4. Summary

A very sharp boundary between erosion and deposition zones on W and Ta surfaces, similar to the surface observations, is reproduced by using the modified EDDY code. Different chemical erosion yields used in the calculation, e.g., ~0.01 for W and <0.005 for Ta, fitted the calculated widths of the deposition area to the observed values. The higher surface temperature and higher deuterium trapping rate of Ta were possible reasons for the suppressed chemical erosion of the deposited C on Ta.

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