THE RELATIVE IMPORTANCE OF SURFACE
PHENOMENA IN CTR FIRST-WALL DESIGNS

By

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ABSTRACT

Plasma-wall interactions are modeled using physical sputtering theory. Sputtering yields are calculated for incoming D-T ions that have a monoenergetic or Maxwellian distribution in energy. The yield curves assuming the Maxwellian energy distribution are flatter than the monoenergetic curves. The consequences of sputtering considered here are surface composition and microtopography changes of the first-wall surface. For the iron-carbon system, the surface becomes enriched with carbon when deuterons are incident on the target. The number of cycles for crack initiation at the first-wall surface is linearly proportional to differences in sputtering yield of two adjacent areas. These effects are of first order and appear to be dominant in limiting the life of the first wall.

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INTRODUCTION

Plasma-surface interactions that pertain to the first wall of a fusion device have been investigated extensively by numerous workers [1]. Some of the phenomena that have received attention are sputtering, gas desorption, minor constituent buildup in the surface region, and hillock growth and faceting as a result of preferential sputtering. The relative importance of these phenomena, based on their influence on both structural integrity and plasma contamination, has not always been clear and has changed as new experimental data become available. In the present report, we assess the importance of these phenomena after modeling the physical sputtering of heavy targets by light ions. The sputtering yields are calculated for mono-energetic particles and for particles that have a Maxwellian distribution in energy. We utilize these calculated yields to compute surface compositional and microtopography changes and assess the magnitude of these effects on mechanical properties.

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Sputtering by Light Ions

The sputtering theory of Sigmund [2] is used as the basis for the yield calculations. This theory, as originally formulated, is not adequate to describe the sputtering due to light ions; therefore, modifications such as the approach of Schiøtt [3] have been incorporated. We shall not go into the details of the model here [4], except to say that electronic losses are especially important for light ions in the intermediate and low-energy regimes, since they significantly affect the calculated yield values. The inclusion of these losses in the low-energy regime results in an increase in sputtering yield, in contrast to the yield obtained when electronic losses are excluded, since the damage is deposited closer to the surface. At high energies, the yield decreases, since a smaller proportion of the energy goes into damage production. The results of the calculation for deuteron ions sputtering four target materials is shown in Fig. 1. The ordinate is the sputtering yield (S) in atoms per ion and the abscissa is the energy (E) of the monoenergetic deuteron beam. The materials C, Be, and Al were chosen as representative low atomic number (Z) materials, and Fe was chosen because it is the major component of stainless steel.

The sputtering yields are calculated in the following manner: (1) the energy at which S is maximum (E_{max}) is computed from the Kinchin-Pease theory [5], (2) using Sigmund's theory with electronic losses, the S versus E curve is computed, and the yield curve is obtained for $E < E_{\text{max}}$ (dashed line) and $E > E_{\text{threshold}}$, where $E_{\text{threshold}}$ is the threshold energy estimated by Houston [6], and (4) the yield curve for $E < E_{\text{max}}$ is shifted so that its value of S at E_{max} coincides with that for the $E > E_{\text{max}}$ curve. These results show that the yields go through a maximum, which is in the 10^{-1} range, and the maximum shifts to higher energies as the atomic number of the target increases. Similar

curves for tritium ions, alpha particles, and protons have been obtained [4].

The first wall of a CTR will experience bombardment by light ions that have a broad energy distribution. The erosion rates of first-wall materials may be obtained by "folding in" the energy distribution with the yield calculation. If we assume, for example, a Maxwellian energy distribution, the erosion rates may be calculated as a function of the average energy of the incoming particles. Figure 2 shows the results for a monoenergetic or a Maxwellian distribution of deuteron ions incident on Fe or Be. For the Maxwellian distribution, the abscissa is the average energy of the distribution ($3/2 kT$). The sputtering yield curves are flattened out when the energy distribution is included in the calculation.

Surface Composition and Microtopography Changes Due to Preferential Sputtering

The changes in surface composition for a two-component system may be modeled when the sputtering yields versus energy are known. We follow the approach of Shimizu, et al. [7] for the steady-state sputtering of a two-component alloy. The assumption is made that monoenergetic particles are incident on the target and that all atoms sputter independently. The changes in surface composition are obtained from a knowledge of the ratio of the sputtering yield for the pure elements to their bulk compositions. The results of the calculation using this model are shown in Fig. 3. The sputtering of a compound composed of a homogeneous mixture of iron and carbon by a monoenergetic D^+ beam was considered. The ratio of sputtering yields of Fe to C was obtained from Fig. 1 and inserted into an expression that relates surface concentration, sputtering ratio and bulk composition. The bulk concentration of carbon was taken as 1 at.%. The surface concentration of carbon increases dramatically with energy since the ratio of sputtering yields increases with energy. The surface becomes enriched with Fe for energies lower than ~1 keV, whereas above this value a carbon-rich surface would be

expected. This model predicts order-of-magnitude changes in one or the other of the components in which solubility limits will have been exceeded. The surface composition changes will not only influence the yields by modifying the surface-energy term in the sputtering theory but will also affect the mechanical properties of the first wall.

The effects of preferential sputtering will lead to roughening of the first-wall surface. Assuming the surface is composed of regions of material that have different sputtering coefficients ($S_2 - S_1 = \Delta S$) for a given dose rate, an average surface roughness R will be produced. The number of cycles for fatigue crack initiation has been shown to be related to the average surface roughness that was mechanically produced for Type 304 stainless steel for a given set of experimental conditions [8]. Making use of these facts, the relationship between the number of cycles for crack initiation, N_0 , caused by thermal cycling and the difference in sputter yield, ΔS , can be established (Fig. 4). For differences in yield of 0.1 (10%) between two grains, for example, the number of cycles for crack initiation is $\sim 10^3$. The time for crack initiation, assuming a 1-min cycle time as proposed for the ANL/TEFR [9], is $\sim 10^3$ min.

It should be noted that the absolute numbers of the ordinate are correct only in the context of the approximations contained in the model. For example, a direct relationship between thermal cycling and the strain-controlled fatigue tests used in deriving the relationship between N_0 and R has not been established. Furthermore, crack propagation and initiation will exhibit different behavior in composite structures when compared with one-component materials. However, the calculations do show that surface roughening caused by sputtering can significantly affect the useful life of a CTR first-wall.

In summary, wall-erosion calculations should include the distribution in energy of the incoming particles. Surface concentration and microtopography

changes of the first wall are of primary importance when the mechanical response is considered.

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LIST OF FIGURES

- Fig. 1.** Yield vs energy for deuteron ions impinging on Be, Al, C, and Fe. The solid line is the result of the calculation using the modified Sigmund theory. The slope of the dashed line, computed from Sigmund's theory, is based on sputtering data for low-energy incoming particles and is drawn to coincide with the solid line at the maximum yield, which was calculated using the Kinchin-Pease model.
- Fig. 2.** Yield vs energy for deuteron ions impinging on Be and Fe. The dashed curve shows yields for monoenergetic ions, whereas the solid curve shows the yield for a Maxwellian distribution in energy. In the latter case, the energy scale is the average energy of the Maxwellian.
- Fig. 3.** The surface concentration of carbon vs the energy of the deuteron ion beam. An alloy composed of Fe and C was chosen, with a 1 at.% bulk concentration of carbon.
- Fig. 4.** The number of cycles for crack initiation vs the difference in yield. The number of cycles are converted to time, assuming a 1-min cycle time as proposed for the ANL/TEPR.

SURFACE CONCENTRATION (PERCENT CARBON)

NUMBER OF CYCLES FOR CRACK INITIATION

TIME FOR CRACK INITIATION (TEPR DESIGN), IN MINUTES