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Dependence of Sputtering Erosion on Fuel-Pellet Characteristics

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by

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ABSTRACT

Conceptual designs of fusion reactors operating on the principle of inertial confinement require that the dependence of cavity-wall erosion on fuel-pellet energy yield, its mass, and representative atomic number be known. A simple approximate model of sputtering erosion is presented and explicit formulae are derived that express the total amount of eroded wall material in terms of the above three parameters.

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INTRODUCTION

An approximate model and its analysis are described, which lead to explicit formulae that estimate trends in sputtering erosion without detailed calculations. These results will be useful in parametric studies of conceptual fusion reactor designs operating on the principle of inertial confinement. For such studies, the dependence of total eroded wall material on the atomic number (Z), of impinging ions on total pellet mass (M), and on its energy yield (Y) must be known. Such knowledge will aid in the selection of desirable materials for structural shells of fuel pellets.

Detailed calculations of sputtering erosion in reactor cavity walls and their application to the conceptual design of fusion reactors have been described previously.¹ In our present study we approximated the sputtering yield and calculated the erosion explicitly. The model used in the analysis is described, and calculations, results, and conclusions are presented.

THE SPUTTERING MODEL

The sputtering model contains two parts: (a) the dependence of the sputtering coefficient S on the energy E of impinging ions, and (b) the dependence of ion fluence N on fuel-pellet mass M and on its other characteristics.

Sputtering Coefficient $S(E)$

To derive the parametric dependence of sputtering erosion we postulate that the sputtering coefficient S depends on ion energy E in the following manner.

- $S(E)$ increases linearly from zero at $E = 0$ to S_m at E_m , where S_m is the maximum value of S and E_m is the ion energy at which sputtering is highest;
- $S(E)$ remains constant in the region $E_m \leq E \leq rE_m$, where $r \geq e$ is an arbitrary constant (the restriction on r is not essential and will be explained later); and
- $S(E)$ decreases as $\ln \epsilon / \epsilon$ for $E \geq rE_m$ where $\epsilon = E/E_m$ is the nondimensional ion energy.

This behavior, represented schematically in Fig. 1, is a reasonable approximation to the theoretically and experimentally determined functional dependence $S(E)$.^{1,2} In our approximation we assumed that the threshold energy is practically zero, which is satisfactory for our analysis because this energy is usually less than 10 eV and therefore negligible in comparison to E_m , which generally equals tens or hundreds of keV.

The physical quantities E_m and S_m are characteristic of ion material and depend on its atomic number Z ; we use Sigmund's theory³ to calculate that dependence. The results for molybdenum and carbon targets (walls) are shown in Figs. 2, 3, 4,

Fig. 1. Model of sputtering yield.

and S ; they indicate that $E_m(Z)$ is nearly quadratic and $S_m(Z)$ nearly linear in Z . Accordingly we set:

$$E_m = KZ^2 \quad (1)$$

$$S_m = C_1 + C_2Z, \quad (2)$$

where the constants K , C_1 , and C_2 are obtained by matching Eqs. (1) and (2) with theoretically or

Fig. 2. Location of maximum sputtering, S_m , for a molybdenum target.

Fig. 3. Maximum of sputtering coefficient for a molybdenum target.

Fig. 4. Location of maximum sputtering, S_m , for a carbon target.

Fig. 5. Maximum of sputtering coefficient for a carbon target.

experimentally obtained dependencies $E_m(Z)$ and $S_m(Z)$. For example, a molybdenum target (wall), Figs. 2 and 3 indicate $K \approx 9000$, $C_1 \approx 2.0$, and $C_2 \approx 0.2$.

Consistent with the approximations inherent in Eqs. (1) and (2) we also approximate the atomic weight, a , by:

$$a = 2Z + \delta Z^2, \quad (3)$$

where δ has a small constant value.

Ion Fluence N

In our parametric analysis we assumed that the pellet composition can be characterized with adequate accuracy by an average atomic weight, a . Consequently, the number of plasma ions generated in its microexplosion is:

$$N = \frac{MA}{a}, \quad (4)$$

where $A = 6.023 \times 10^{23}$ atoms/mole is Avogadro's number. If we further assume that the yield

energy is uniformly distributed over all the ions then the average energy per ion, E , is given by:

$$E = \frac{fYa}{MA}, \quad (5)$$

where Y is the total microexplosion yield energy in eV, and f is the fraction of yield deposited in plasma debris.

ANALYSIS AND RESULTS

As stated in the Introduction, the objective of our analysis is the calculation of the total amount of material eroded from the cavity wall of an inertial confinement fusion reactor, given by:

$$E_r = S \cdot N. \quad (6)$$

The three ion-energy regimes--low, intermediate, and high--in which the sputtering coefficient either increases, remains constant, or decreases will be considered separately.

Low-Energy Regime, $E \leq E_m$

Plasma ions will be in the low-energy regime when the inequality $(fYa/MA) \leq E_m$ is satisfied; in general, this is true when the pellet yield-to-mass ratio is low.

In this regime sputtering yield increases linearly with ion energy and therefore is given by $S = (S_m/E_m)E$. Using this expression together with Eqs. (4) and (5) in Eq. (6) we obtain

$$E_r = \frac{S_m}{E_m} fY, \quad (7)$$

which upon substitution of expressions for E_m and S_m [Eqs. (1) and (2), respectively] becomes

$$E_r = \frac{C_1 + C_2 Z}{KZ^2} fY.$$

This result shows that in the low-energy regime (where the sputtering coefficient increases with ion energy) the total amount of material eroded is independent of pellet mass; is directly proportional to the total ion energy; and, for a constant yield, decreases with increasing atomic number, Z , of the pellet material.

Intermediate-Energy Regime, $E_m \leq E \leq rE_m$

In this regime, the ion energy satisfies the inequalities $E_m < (fYa)/(MA) \leq rE_m$ and the sputtering coefficient does not change with ion energy. Consequently, the amount of eroded material is given by:

$$E_r = S_m \frac{MA}{a} \quad (8)$$

By using Eqs. (2) and (3) to express E_r in terms of atomic number we obtain:

$$E_r = \left(\frac{MA}{Z} \right) \frac{C_1 + C_2 Z}{2 + \delta Z}.$$

This result shows that in the intermediate-energy regime (where the sputtering coefficient is independent of ion energy) the amount of eroded material does not directly depend on fuel-pellet energy yield; is proportional to pellet mass, M ; and for constant M decreases with increasing Z . The decrease, however, may not be uniform for some combinations of values for C_1 , C_2 , and δ .

High-Energy Regime, $E > rE_m$

Plasma ions are in the high-energy regime when the inequality $(fYa/MA) > rE_m$ is satisfied; in general this is true when the pellet yield-to-mass ratio is high.

Theoretical and experimental investigations indicate^{2,3} that in the high-energy regime the sputtering coefficient decreases with increasing energy as ϵ^{-1} (this function decreases monotonically for $\epsilon \geq e$, hence the previous restriction on r); consequently:

$$S = \frac{r S_m}{f n r} \frac{\ln \epsilon}{\epsilon},$$

where the multiplicative constant was determined from the continuity of S at $E = rE_m$.

Substituting the above expression for S together with Eqs. (4) and (5) into Eq. (6) we obtain:

$$E_r = \frac{r(MA)^2 E_m S_m}{f Y f n r a^2} \ln \frac{f Y a}{MA E_m} \quad (9)$$

In this expression the product $E_m S_m$ increases as Z^3 [Eqs. (1) and (2)] and a^2 increases as Z^2

[Eq. (3)]. However, no convenient estimate exists that would reflect the variation of the logarithmic term with Z . The following considerations indicate the behavior of E_r . For low Z values E_m is relatively small making the argument of the logarithm large and the logarithm itself slowly varying with Z . Thus the behavior of E_r is determined predominantly by the factor $E_m S_m / a^2$, which increases with Z . For high values of Z the argument of the logarithm decreases as a constant divided by Z and the logarithm itself diminishes more rapidly than the increasing factor $E_m S_m / a^2$. Thus, E_r eventually begins to decrease with increasing Z .

To verify the above deduced behavior and to obtain an idea of the value of Z at which E_r changes from an increasing to a decreasing function of Z we have evaluated Expression (9) numerically by using exact expressions from Sigmund's theory for $E_m(Z)$ and $S_m(Z)$,³ and exact values from the periodic table of elements for $a(Z)$. The calculation was carried out for $r = 2.80$, $f = 0.20$, $Y = 100$ MJ, and $M = 0.07$ g chosen so that ions are in the high-energy regime for all values of $Z \leq 48$.

The result is plotted in Fig. 6. It shows that E_r behaves as predicted: Initially increases with Z , reaches a maximum (at $Z = 8$ for the particular set of parameter values used in this sample computation), and then decreases as Z increases. The curve is extended beyond $Z = 49$ to illustrate the trend. The behavior, however, is not uniformly smooth but shows small undulations in the general trend near the maximum.

CLOSING COMMENTS

The analysis presented in this report led to expressions that estimate the total amount of eroded wall material for different impinging ions in terms of ion atomic number and other parameters characterizing ion fluence. The complementary problem of determining amounts of different wall materials eroded by a given ion flux has been investigated extensively by Wehner and his collaborators^{4,5,6}. Their findings are summarized in Sec. 7.4.2 of Ref. 2; the results presented in convenient graphical form may be found on pp. 315-316 and need not be reproduced here. Briefly, the

Fig. 6. Total sputtering erosion in the high-ion-energy regime.

sputtering yield follows closely, with minor exceptions, the state of electron concentrations in the "d" shells of target (wall) material atoms and also crudely resembles the reciprocals of the heats of sublimation. Thus the yield varies almost periodically with target atomic number.

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