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A PHYSICAL SPUTTERING CODE FOR FUSION APPLICATIONS*

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Abstract

A computer code, DSPUT, has been developed to compute the physical sputtering yields for various plasma particles incident on candidate fusion reactor first-wall materials. The code, which incorporates the energy and angular-dependence of the sputtering yield, treats both high- and low-Z incident particles bombarding high- and low-Z wall materials. The physical sputtering yield is expressed in terms of the atomic and mass numbers of the incident and target atoms, the surface binding energy of the wall materials, and the incident angle and energy of the particle. An auxiliary code has been written to provide sputtering yields for a Maxwellian-averaged incident particle flux. The code DSPUT has been used as part of a Monte Carlo code for analyzing plasma-wall interactions.

Introduction

Physical sputtering of first-wall materials by energetic plasma particles is expected to be a major source of plasma contamination in fusion power reactors. As a result, the achievement of satisfactory plasma performance will be dependent, to a large extent, upon the proper selection of the first-wall material for the appropriate plasma edge conditions. Although the mean plasma temperature in a tokamak reactor will be of the order of 10 keV, the plasma edge temperature is expected to be substantially lower. Depending on the methods of burn control, plasma heating, fueling, and impurity control, the plasma edge temperature and the mean incident particle energy may vary from the order of 10 eV to a few keV. A comprehensive physical sputtering model is needed for incorporation into plasma-wall interaction models to evaluate the behavior of the plasma edge region and the overall plasma performance.

Considerable physical sputtering data generated within the last few years (see Refs. 1-6 for summaries) provide a basis for upgrading earlier physical sputtering models (2,6-9). In the present investigation, a computer code, DSPUT, has been developed to compute the physical sputtering yields for various plasma particles incident on candidate fusion reactor first-wall materials. The code, which is an upgrade of an earlier model (6,7), incorporates the energy and angular dependence of the sputtering yield for both high- and low-Z particles incident on high- and low-Z wall materials. An auxiliary code provides sputtering yields for a Maxwellian-averaged incident particle flux. The DSPUT code is used as part of a Monte Carlo code for analysing plasma-wall interactions.

Sputtering Model

The sputtering model incorporates recent information on physical sputtering into an analytical expression that gives the sputtering yields of various wall materials as a function of the energy and angle of the incident plasma particles.

$$S(E,\theta) = S(E)\, S(\theta) \qquad (1)$$

The sputtering yield is expressed in terms of the atomic and mass numbers of the incident particles and wall materials, energy and angle of the incident particles, binding energy of the wall atoms, and appropriate constants.

Energy Dependent Function

The energy dependent term $S(E)$ is similar in form to the model developed previously (6,7). The experimental data base, particularly for the energy dependence of light-ion sputtering, has been greatly expanded. Much of these data are summarized in Refs. 1-6. Data from several investigators were used as a basis for the model. In many cases, significantly different sputtering yields have been reported by different investigators for supposedly identical conditions. In these cases, the data were evaluated with respect to consistency of the yields for different incident particles and wall materials. For example, the H/D and the D/He sputtering yield ratios were compared. Potential chemical effects, such as hydride formation and oxygen contamination, were considered. In the case of beryllium and aluminum, for example, the experimental yields for the metals and oxides are unexpectedly similar (2). These results are probably affected by oxygen contamination of these highly active metals. To the degree possible, data were selected from wall materials with a wide range of mass numbers. Much of the data for the heavy ion sputtering are from the noble gases.

The earlier model for the energy dependent sputtering yield was modified to the following expression:

$$S(E) = \frac{C}{U_0} Z_1^{0.75} (Z_2 - 1.8)^2 \left(\frac{M_1 - 0.8}{M_2}\right)^{1.5} \frac{(E - E_{th})}{(E - E_{th} + 50 Z_1^{0.75} Z_2)^2} , \qquad (2)$$

where

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C = 2000 for incident hydrogen
  = 400 for all other particles
U_0 = binding energy of wall material, eV (see Table 1)
Z_1 = atomic number of incident particle
Z_2 = atomic number of wall material
M_1 = mass number of incident particle
M_2 = mass number of wall material
E = energy of incident particle, eV
E_{th} = threshold energy for sputtering of system given by Eq. (3).

The threshold energy for sputtering is given by

$$E_{th} = \frac{(4M_1 + M_2)^2}{4M_1M_2} U_0. \quad (3)$$

The atomic and mass numbers and the binding energy values for several wall materials are listed in Table 1.

Table 1. Parameters for Calculation of Physical-Sputter Yields for Several Wall Materials

Wall Material	Z	M	U_0,eV
Be	4	9.0	3.4
B	5	10.8	5.7
C	6	12.0	7.4
Al	13	27.0	3.4
Si	14	28.1	4.7
Ti	22	47.9	4.9
V	23	50.9	5.3
Fe	26	55.9	4.3
Ni	28	58.7	4.4
Nb	41	92.9	7.6
Mo	42	95.9	7.8
Ta	73	180.9	10.4
W	74	183.9	11.1

The sputtering yields given by the model are considered representative of those for all incident particles incident on all single element wall materials with the possible exception of the group 1 B elements. These elements (viz., copper, silver, and gold) generally produce slightly higher yields relative to other materials than one might predict. Experimental data (1,2) indicate that sputtering yields for iron- and nickel-base alloys are similar to those for pure iron and nickel, respectively. Therefore, one can use the model, with a reasonable degree of confidence, to predict the sputtering yields of many alloy systems if a binding energy value can be obtained.

Angular-Dependent Function

The data base for development of an angular-dependent function is much more limited. Most of the data are summarized in Refs. 2, 9, and 10. Based on these limited data, the angular-dependent function can generally be represented by some type of a cosine distribution (2,9). The experimental data indicate that the angular-dependent function varies significantly with incident particle, incident particle energy, and wall material. The following expression provides a good empirical fit to the available data.

$$S(\theta) = \cos^{-f}(\theta) \quad (\theta \text{ in degrees}) \quad (4)$$

where

$$f = \frac{1}{(20Z_1)^{0.5}} \left(\frac{M_2}{M_1}\right)^{0.25} (E - 4E_{th})^{0.25} \left(1 - \frac{\theta}{90}\right)^{0.5} \quad (5)$$

The parameters Z_1, M_2, M_1, E, and E_{th} are defined in Eq. (2) and θ is in degrees. This expression is suggested for

$E > 4E_{th}$

$0 \leq \theta < 89^0$

for $E < 4E_{th}$, $S(\theta) = 1$. Since $S(\theta)$ should go to 0 as θ approaches 90^0, a discontinuity with $S(\theta) = 0$ is proposed for $\theta > 89^0$. For most cases with an angular distribution of incident particles, very little difference would be obtained if Eqs. (4) and (5) were assumed valid over the total range of 0 to 90^0.

Since the angular-dependent function is an empirical equation based only on light-ion (H, D, and He) data for energies < 10 keV, the validity of this expression for higher energy or higher mass number incident particles is uncertain. The model gives a relatively good representation of the available data for single element wall materials and should provide a reasonable approximation of the angular effect for light ions with energies < 10 keV incident on most wall materials.

Code

The model described has been incorporated into a fortran code DSPUT. Because of the relative simplicity of the analytical model, the code is fairly short and fast running (~250 μs per call on IBM 370-195). Figures 1 through 3 are plots of the monoenergetic sputtering yields as a function of energy for deuterium, helium, and self-ions, respectively, incident on beryllium, graphite, stainless steel (Fe), molybdenum, and tungsten. Figure 4 is a plot of the angular dependence of the sputtering yield for deuterium at energies of 0.4, 1, and 2 keV incident on nickel.

Application

As an example of the application of the DSPUT code, a computation was made for the erosion of an INTOR-type divertor. This used the computer code DEGAS (11) which models neutral transport in tokamak divertors and limiter designs using Monte Carlo methods. Neutrals are typically produced by plasma ions streaming into a neutralizing plate where they reflect or desorb as atoms or molecules. The code follows test particles representing these neutral particles through charge exchange, ionization, dissociation, and wall collisions (Fig. 5). Plasma conditions are assumed to remain unchanged during the flight. Ionization and charge exchange rates are recorded from these flights as well as wall interactions and gas flow rates.

In particular, at each collision with a wall, a call is made to DSPUT with the test particle energy and incident angle. A sum, $S = \Sigma w.s$, is tallied over all collisions for each wall segment, where w is the number of real particles/sec.cm the test particle represents, and s is the sputtering coefficient outputted from DSPUT. When all test flights have been flown, dividing S by the segment length gives the number of atoms of wall material sputtered per second per cm^2. Converting by the factor $3.76 \times 10^{-16} s.cm^3/yr.atom$ gives the result in cm/yr.

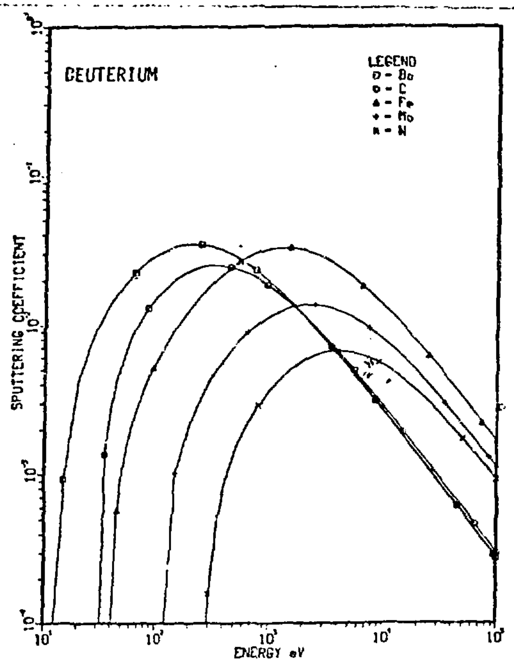

Fig. 1. Calculated energy-dependent physical sputtering yields for candidate wall materials bombarded with normally-incident monoenergetic deuterium.

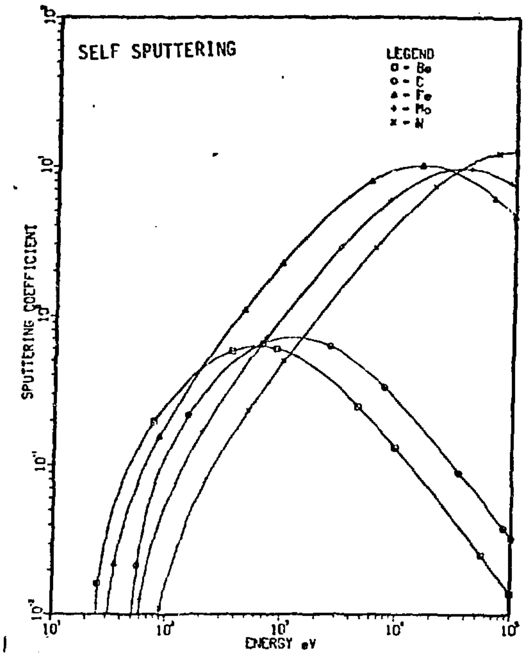

Fig. 3. Calculated energy-dependent self-sputtering yields for candidate wall materials (normal incidence, monoenergetic).

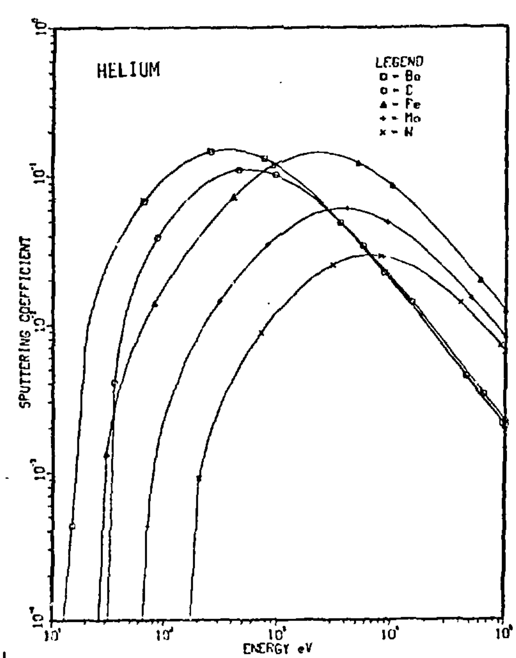

Fig. 2. Calculated energy-dependent physical sputtering yields for candidate wall materials bombarded with normally-incident monoenergetic helium.

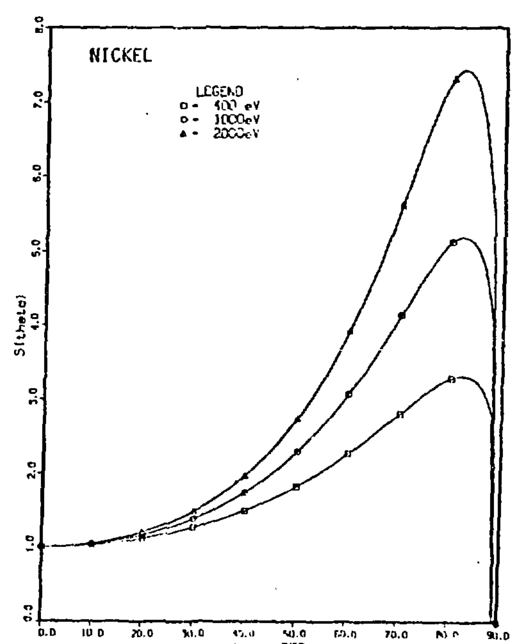

Fig. 4. Calculated angular-dependent physical sputtering yields for 0.4, 1.0 and 2.0 KeV deuterium incident on nickel (normalized to normal incidence).

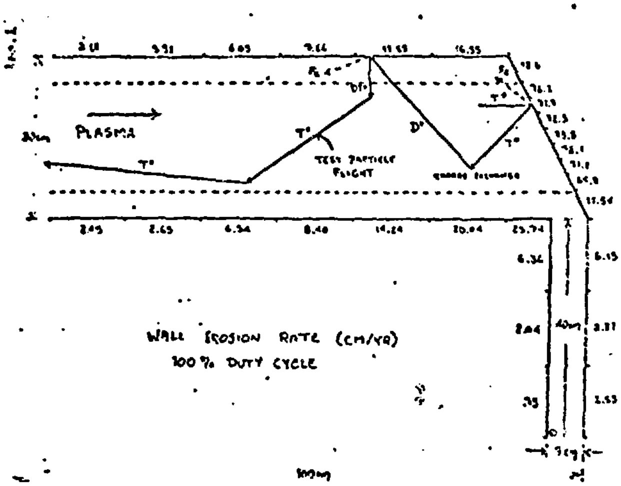

Fig. 5. Calculated wall erosion rate in cm/yr for an INTOR divertor assuming a 100% duty cycle. Plasma is 47.5% D, 47.5% T, and 5% He, with constant ne = 3.31e12, T = 250 eV. Flow is of the plasma sound speed in a direction 8 degrees from the normal of the poloidal plane. Sheath potential is 3xT. Petravic [12] has shown that high density, low temperature regimes are possible, resulting in much less erosion than shown here.

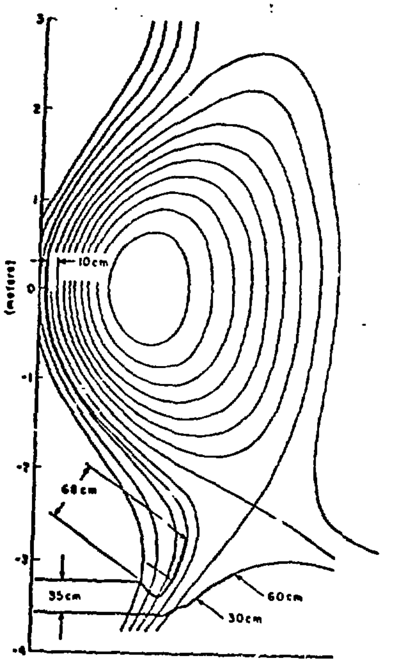

Fig. 6. Poloidal cross-section of proposed INTOR poloidal divertor configuration (from "International Tokamak Reactor, Phase-1," IAEA, Vienna (1981).

Results from a sample calculation for an INTOR-type divertor (Fig. 6) are given in Fig. 5. A plasma of constant ne = 3.31×10^{12} and T = 250 eV, consisting of 47.5% D, 47.5% T, and 5% He flows into the 100 x 30 cm device at the plasma sound speed, in a direction 8 degrees from the normal of the poloidal plane. At the neutralizing plate, the ions fall through a sheath potential taken to be 3xT = 750 eV. The results show peak erosion rates of about 78 cm/yr at the plate for a 100% duty cycle if no redeposition of sputtered material is assumed. This shows the need for operating the divertor in regimes where the temperature at the plate is considerably lower than 750 eV. Petravic (12), in a self-consistent calculation using fluid model incorporation DEGAS, has shown that such regimes may be possible.

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