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The Effect of the Angular Dependence of Sputtering in Fusion Reactors

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Abstract

Recent work on the angular distribution of sputtering yields is reviewed and then compared with experiment. The most probable angular distribution law is evaluated from experiment. By averaging over an incident Maxwellian spectrum of ions, it is shown that there is considerable enhancement over the isotropic case, which would increase the total sputtering at the walls or limiters of fusion reactors over the example of an isotropic angular distribution.

1. Introduction

It is generally accepted that the principal source of impurities likely to cause excessive radiation losses in fusion reactors will be the sputtering of ions from the wall and limiters of fusion reactors. A review of available experiments for light ions incident normal to a range of surfaces was given by Thomas *et al.* (1979); further, Matsunami *et al.* (1980*a*), Berische (1981), Cook *et al.* (1982) and Langley (1984) analysed the Thomas *et al.* data to find a set of semi-empirical laws which describe both the energy dependence and the scaling laws for the constants involved. In fusion reactors, however, the ions incident on the appropriate surface will have an approximate Maxwellian distribution of energies, and an isotropic incidence on the surface. The question then arises as to how the sputtering rate varies with respect to the angle the incident ion makes with the normal to the surface. This was first investigated theoretically by Winterbon *et al.* (1970) and reviewed recently by Yamamura *et al.* (1983*a*) in relation to the reflection coefficient. Yamamura *et al.* (1983*b*) derived the following expression for light ion sputtering at normal incidence:

$$Y(E) = 0\cdot042\,\frac{F_{\mathrm{D}}(E^*)\,R_{\mathrm{N}}(E)}{U_{\mathrm{S}}}\{1-(E_{\mathrm{T}}/E)^{\frac{1}{2}}\}^{2\cdot8}, \tag{1}$$

where $F_{\mathrm{D}}(E^*)$ is the energy deposited near the solid surface by a backscattered ion, E^* is the average energy of the reflected ion, and $R_{\mathrm{N}}(E)$ is the particle reflection coefficient of the ion with incident energy E. The surface binding energy is U_{S}, while E_{T} is the sputtering energy threshold for normal incidence. Other formulae have been given by Bohdansky (1984) and Matsunami *et al.* (1980*b*).

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For incident ion angles not too far from the normal, the normalized angular dependence is found from the equation

$$\frac{Y(E,\theta)}{Y(E,0)}=\frac{F_{\mathrm{D}}(E^*(\theta))}{F_{\mathrm{D}}(E^*(0))}\,\frac{R_{\mathrm{N}}(E,\theta)}{R_{\mathrm{N}}(E,0)}\,. \tag{2}$$

The angular dependence of the reflection coefficient is given by the ion range distribution in the solid. For small angles of incidence, Winterbon *et al.* (1970) showed that if θ is the angle to the normal, then

$$R_{\mathrm{N}}(E,\theta)/R_{\mathrm{N}}(E,0)=(\cos\theta)^{-f}\,, \tag{3}$$

where for a large mass ratio of target to ion $f\approx 2$. Yamamura *et al.* (1983*a*) argued that E^* is only weakly dependent upon θ, so for small θ we have

$$Y(\theta)/Y(0)\approx(\cos\theta)^{-f}\,. \tag{4}$$

As the angle of incidence becomes larger, the effect of surface channelling begins to intrude. To sputter target atoms from the first atomic layer, the ion must penetrate along this layer and this makes absorption more probable. The attenuation of the beam is given by

$$P(\theta)=\exp(-N\sigma R_0/\cos\theta)\,, \tag{5}$$

where σ is the microscopic absorption cross section, N is the number density in the surface layer, and R_0 is the lattice constant, given by $N^{-\frac{1}{3}}$.

Combining the small angle law (3) with the large angle law (4), Yamamura *et al.* (1983*a*) proposed the distribution

$$Y(E,\theta)/Y(E,0)=t^{f}\exp\{-\beta(t-1)\}\,, \tag{6}$$

where $t=1/\cos\theta$ and $\beta=N\sigma R_0$. The angle of incidence of the maximum yield in equation (6) is

$$\theta_{\max}=\cos^{-1}(\beta/f)\,. \tag{7}$$

Much of the experimental data is contained in unpublished reports, although Yamamura *et al.* (1983*a*) fitted equation (6) very well to the published data of Oechsner (1973), Bay and Bohdansky (1979), Bay *et al.* (1980) (see also Bohdansky 1984) and Bohdansky *et al.* (1982). From their fits, it is clear that equation (6) is a very satisfactory description of the observed distributions.

Table 1. Values of distribution constants

E (keV)	θ^0_{max} Fit	θ^0_{max} Calc.	f Fit	f Eq. (15)	σ[A]	E (keV)	θ^0_{max} Fit	θ^0_{max} Calc.	f Fit	f Eq. (15)	σ[A]
			Ni+ H						*Cu+ H*		
0·45	74·4	79·3	1·62	2·22	1·84	0·50	82·1	86·6	1·88	9·41	0·61
1·0	78·3	81·2	2·34	3·20	1·51				*Cu+ He*		
4·0	82·3	83·8	2·27	4·82	1·07	1·05	66·5	65·8	1·55	1·24	4·27
0·45	78·7	79·3	2·19	2·22	1·84				*Mo+ H*		
1·0	82·9	81·2	2·32	3·20	1·51	2·0	81·8	84·0	2·40	4·12	1·31
4·0	84·2	83·8	2·62	4·82	1·07	8·0	82·0	85·8	2·8	6·44	0·93
			Ni+ D						*Mo+ D*		
1·0	80·4	75·5	1·88	1·98	2·49	2·0	82·0	80·1	1·98	2·62	2·17
			Ni+ He						*Mo+ He*		
0·10	56·3	47·6	3·20	0·348	6·71	4·0	77·3	76·2	2·23	1·94	3·0
0·50	66·1	61·6	3·30	0·98	4·72				*Au+ H*		
1·0	72·1	66·1	2·50	1·20	4·02	1·0	78·0	81·7	1·14	0·0	1·90
4·0	79·0	73·1	2·09	1·73	2·89	4·0	79·5	84·1	1·53	4·77	1·35
4·0	80·5	73·1	1·52	1·73	2·80				*Au+ D*		
						1·0	79·2	76·2	1·22	0·0	3·15

[A] Units of σ are 10^{-16} cm^2.

2. Analysis of Data

In Table 1 we give the results of fits to the experiments by Yamamura *et al.* (1983*a*). They also showed that θ_{max} is strongly correlated to stopping power parameters, and gave the law

$$\theta_{max} = 90° - 57 \cdot 3° \eta(E), \tag{8}$$

where

$$\eta(E) = \frac{a}{R_0}\left(\frac{1}{2\epsilon q}\right)^{\frac{1}{2}}, \tag{9}$$

with

$$q = (U_S/\gamma E)^{\frac{1}{2}}, \tag{10}$$

$$\epsilon = E/E_L, \tag{11}$$

$$E_L = \frac{M_1+M_2}{M_2}\,\frac{Z_1 Z_2 e^2}{a}, \tag{12}$$

$$a = 0 \cdot 4685\left(\frac{1}{Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}}}\right)^{\frac{1}{2}}, \tag{13}$$

$$\gamma = 4M_1 M_2/(M_1+M_2)^2, \tag{14}$$

and where Z_1, M_1 are the charge and mass of the projectile and Z_2, M_2 those of the target atom. In Table 1 we show θ_{max} calculated from equations (8)–(14) for a range of ten experiments. The agreement is satisfactory, considering that none of the published graphs contain error bars.

Now we come to a discussion of the power coefficient f. P. L. Smith *et al.* (personal communication 1983) quoted the empirical equation

$$f = 0; \qquad E \leqslant 4E_{\mathrm{T}} \tag{15a}$$

$$= \frac{1}{(20Z_1)^{\frac{1}{2}}}\left(\frac{M_2}{M_1}\right)^{\frac{1}{4}}(E-4E_{\mathrm{T}})^{\frac{1}{4}}; \qquad E > 4E_{\mathrm{T}}, \tag{15b}$$

but it can be seen from the tabulated values in Table 1 that equations (15) do not hold for any of the results by Yamamura *et al.* (1983*b*). Keeping in mind that no error analysis has been carried out on the experiments, and that the theoretical value of f is approximately 2, we postulate that the values of Yamamura *et al.* (1983*a*) follow the normal distribution

$$d_{\mathrm{p}} = \{1/\sigma(2\pi)^{\frac{1}{2}}\}\exp\{(f-\bar{f})^2/2\sigma^2\}, \tag{16}$$

and that the total number of values in any interval (f_1, f_2) would be

$$\Delta n = \tfrac{1}{2}n\left\{\mathrm{erf}\left(\frac{f_2-\bar{f}}{\surd 2\,\sigma}\right)-\mathrm{erf}\left(\frac{f_1-\bar{f}}{\surd 2\,\sigma}\right)\right\}; \tag{17a}$$

$$\mathrm{erf}(x) = \frac{2}{\pi^{\frac{1}{2}}}\int_0^x \exp(-t^2)\,\mathrm{d}t. \tag{17b}$$

Analysing the data, we found that

$$\bar{f} = 2\cdot 00, \qquad \sigma = 0\cdot 454, \tag{18}$$

which confirms the theoretical prediction. Table 2 shows the expected values of Δn from equation (17*a*) for a range of f values. The agreement is good.

Table 2. Predicted number of values

Range of f	Δn	
	Observed	Calculated
1·0–1·5	2	2·304
1·5–2·0	7	6·935
2·0–2·5	7	6·935
2·5–3·0	3	2·304

The result (18) for $\bar{f}$ means that the averaging over angles, which has to be carried out when evaluating the problem for a Maxwellian distribution of ions, is trivial. From equations (6) and (18) we get

$$\int_0^{\frac{1}{2}\pi} \mathrm{d}\theta\,\sin\theta\,Y(E,\theta) = \beta^{-1}\,Y(E,0), \tag{19}$$

where, from equations (7) and (18),

$$\beta = 2\cos\theta_{\max}(E) = 2\sin\eta(E). \tag{20}$$

We suspect that the correlation (8) observed by Yamamura *et al.* (1983*a*) is really

$$\beta = 2\eta(E), \tag{21}$$

but in our numerical evaluation of the Maxwellian averages we used equation (20) to obtain

$$\langle S\rangle = \int_{E_\mathrm{T}}^{\infty} \frac{E^{\frac{1}{2}}}{\beta(E)}\, Y(E,0)\,\mathrm{e}^{-E/kT}\,\mathrm{d}E \Big/ \int_0^{\infty} E^{\frac{1}{2}}\,\mathrm{e}^{-E/kT}\,\mathrm{d}E, \tag{22}$$

where T is the temperature of the ion species in K, and k is Boltzmann's constant.

3. Results and Conclusions

Normally, incident ions are accelerated by a plasma sheath to an approximate Maxwellian distribution of order 3 T. The enhancements obtained from the angular dependence of sputtering over ten isotropic cases are shown in Fig. 1. For the hydrogen ion examples the increase is greatest, and decreases as the incident ion becomes heavier. When the relations (21) and (9) are used together with the integral representation (Gradshteyn and Ryzhik 1965),

$$\int_0^{\infty} x^{\nu-1}(x+\beta)^{-\rho}\,\mathrm{e}^{-\mu x}\,\mathrm{d}x = \frac{1}{\sqrt{\pi}}\left(\frac{\beta}{\mu}\right)^{\nu-\frac{1}{2}} \mathrm{e}^{\beta\mu}\,\Gamma(\nu)\,\mathrm{K}_{\frac{1}{2}-\nu}(\tfrac{1}{2}\beta\mu), \tag{23}$$

where $\mathrm{K}_{\frac{1}{2}-\nu}(x)$ is the associated Bessel function, and by substituting into (22), we get the two cases

$$\begin{aligned}\langle S\rangle_{\text{isotropic}} &= \frac{2}{\pi T^{\frac{3}{2}}}\, A(M_1, M_2)\, E_\mathrm{T}^{\frac{1}{2}} \\ &\times \sum_{n=0}^{\infty} \frac{(n+1)(\frac{1}{2})(-\frac{1}{2})(-\frac{3}{2})\ldots(\frac{1}{2}-n)\{(B+E_T)T\}^{n+\frac{3}{2}}}{E_\mathrm{T}^{n}} \\ &\times \mathrm{K}_{-n-\frac{3}{2}}((B+E_\mathrm{T})/2T),\end{aligned} \tag{24}$$

$$\begin{aligned}\langle S\rangle_{\text{anisotropic}} &= \frac{A(M_1, M_2)}{\pi T^{\frac{3}{2}} C}\, E_\mathrm{T}^{\frac{3}{4}} \\ &\times \sum_{n=0}^{\infty} \frac{(n+1)(\frac{3}{4})(-\frac{1}{4})(-\frac{5}{4})\ldots(-\frac{3}{4}-n)}{E_\mathrm{T}^{n}}\, \mathrm{K}_{-n-\frac{3}{2}}((B+E_\mathrm{T})/2T),\end{aligned} \tag{25}$$

in which

$$C = \frac{a}{R_0}\left\{\frac{E_\mathrm{L}}{2}\left(\frac{\gamma}{U_\mathrm{S}}\right)^{\frac{1}{2}}\right\}^{\frac{1}{2}}. \tag{26}$$

In evaluating this series, we have used the formula by Cook *et al.* (1982)

$$S(E,0) = A(M_1, M_2)(E-E_\mathrm{T})/(E+B)^2, \tag{27}$$

in which $A(M_1, M_2)$ is a scaling constant and B a constant which determines the

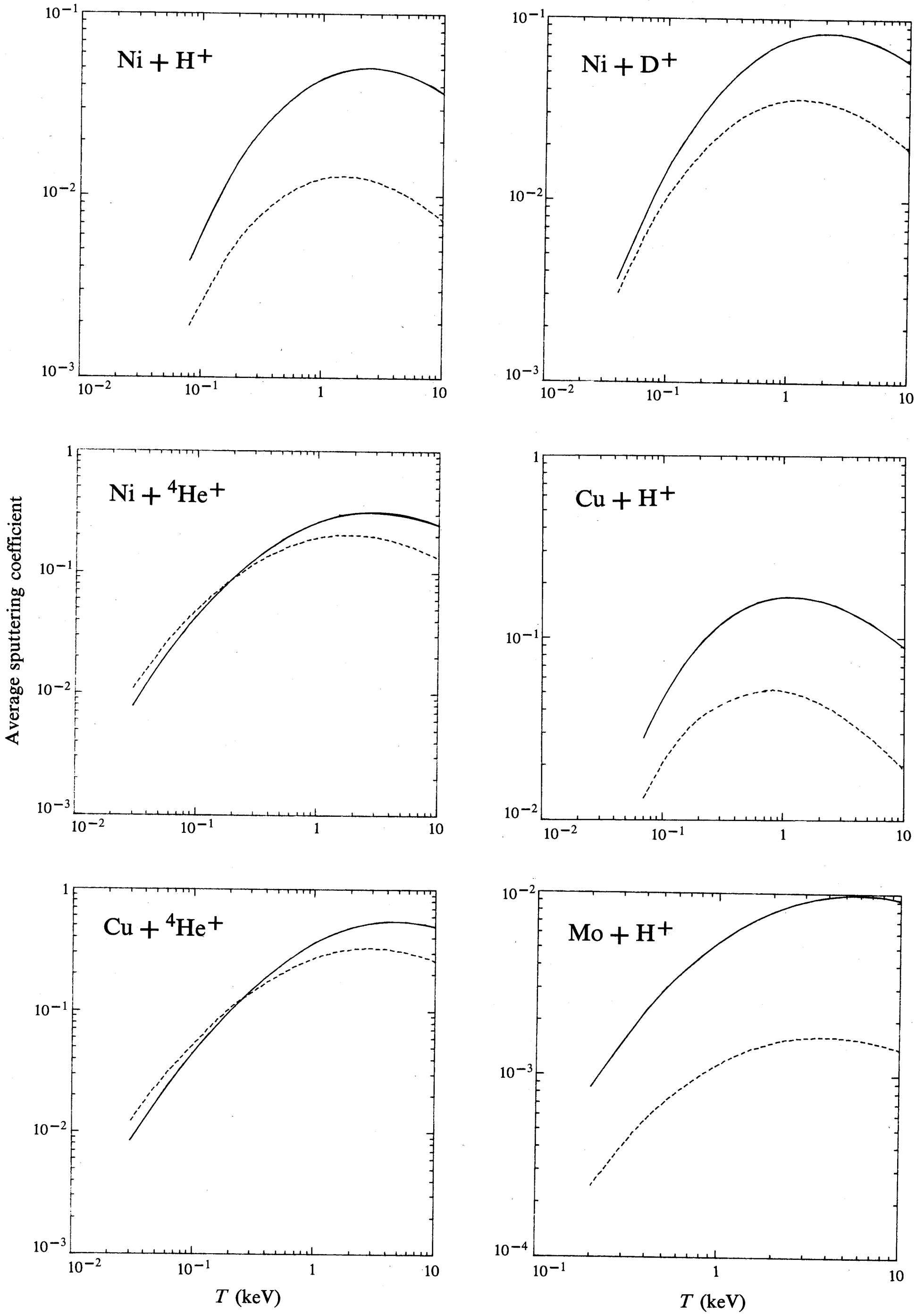

Fig. 1. Comparison between enhanced (solid curves) and isotropic (dashed curves) sputtering for the ten cases indicated.

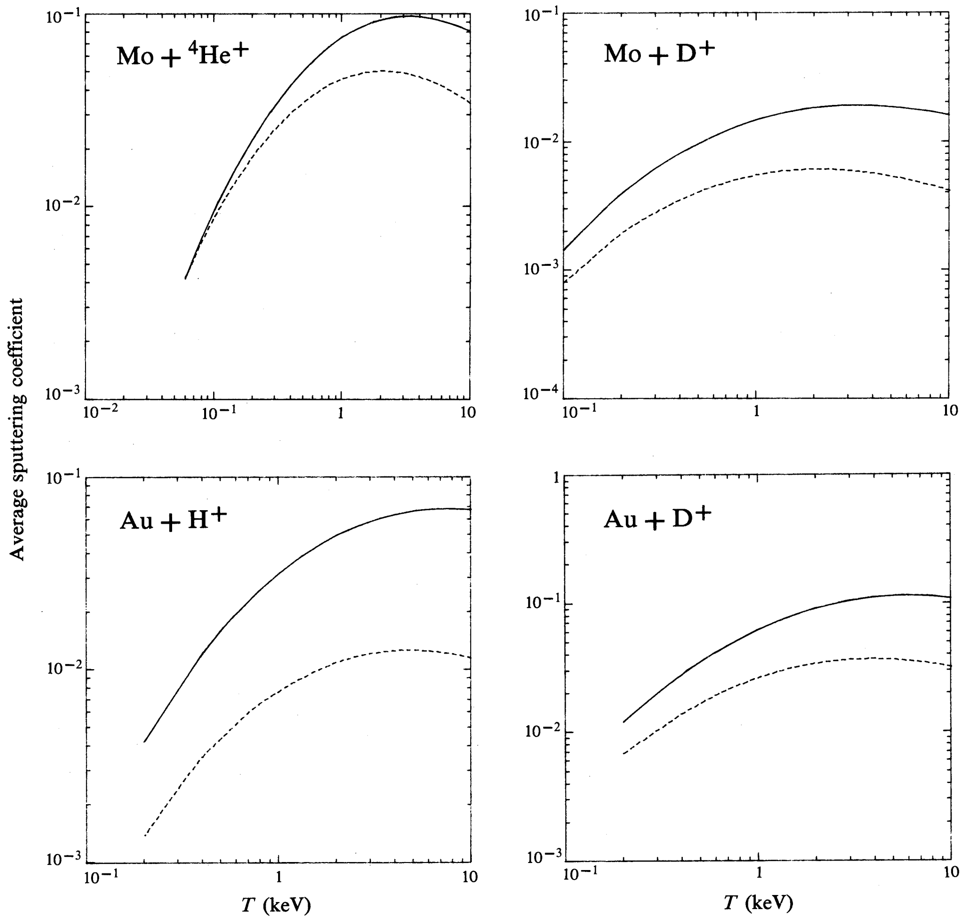

Fig. 1. [*see opposite page*]

maxima of the curves. This series is most useful for large values of T where the convergence is best.

With the theory in its present state, it is possible to predict unmeasured sputtering yields. We propose to carry out a survey of fusion reactor wall conditions and limiter materials to find the combination which would minimize impurity emission into the hot plasma during discharges.

Finally, we note from equations (2) and (9) that the microscopic absorption cross section is given by

$$\sigma = \beta R_0^2,$$

where $\beta = N\sigma R_0$, $N = \rho N_0/M_2$, ρ is the density of the target and N_0 is Avogadro's number. Values of these cross sections are given in the final column of Table 1.

Table 3. Fits of averaged coefficients

Reaction	T_0 (keV)	a_0	a_1	b_0	b_1	b_2	c_0
$C+H^+$	0·08	−1·391	1·296	−3·637	−0·0445	−0·114	0·0632
$C+D^+$	0·10	1·183	1·152	−0·929	−0·132	−0·131	0·831
$C+4He^+$	0·08	0·0222	1·580	−1·927	0·330	−0·177	0·690
$Ni+H^+$	0·2	−2·042	1·343	−3·133	0·330	−0·177	0·209
$Ni+D^+$	0·08	−0·561	1·569	−2·584	0·283	−0·174	0·328
$Ni+4He^+$	0·06	0·486	1·521	−1·358	0·381	−0·173	1·403
$Cu+H^+$	0·1	0·0764	1·374	−1·797	0·0963	−0·165	0·497
$Cu+4He^+$	0·06	0·422	1·479	−1·024	0·521	−0·164	2·790
$Nb+H^+$	0·4	−4·400	1·389	−4·870	0·641	−0·203	0·0648
$Nb+D^+$	0·2	−3·441	1·561	−4·433	0·604	−0·193	0·0971
$Nb+4He^+$	0·08	−1·240	1·779	−2·626	0·840	−0·163	1·172
$Mo+H^+$	0·4	−4·800	1·407	−5·235	0·708	−0·203	0·0523
$Mo+D^+$	0·2	−3·191	1·459	−4·229	0·463	−0·187	0·0891
$Mo+4He^+$	0·08	−0·844	1·644	−2·598	0·454	−0·184	0·454
$W+H^+$	0·8	−6·911	1·126	−6·968	0·699	−0·223	0·00819
$W+D^+$	0·5	−5·821	1·235	−6·080	0·658	−0·202	0·0201
$W+4He^+$	0·6	−3·180	1·194	−3·352	0·752	−0·192	0·402
$Au+H^+$	0·4	−3·017	1·526	−3·468	0·810	−0·208	0·377
$Au+D^+$	0·4	−2·459	1·216	−2·778	0·682	−0·191	0·611
$Au+4He^+$	0·08	0·0921	1·693	−1·568	0·558	−0·183	1·612

In Table 3 we give the results for the coefficients of the fits to the exact numerical integration over the Maxwellian distribution to the forms:

$$E_T < T < T_0; \qquad \ln\langle S\rangle = a_0 + a_1(\ln T),$$

$$T_0 < T \leqslant 10\,\text{keV}; \quad \ln\langle S\rangle = b_0 + b_1(\ln T) + b_2(\ln T)^2,$$

$$T > 10\,\text{keV}; \qquad \langle S\rangle = c_0(T)^{-\frac{3}{4}}.$$

Impurity–impurity sputtering in plasmas is worthy of further investigation.

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