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A Semi-empirical Law for Sputtering in Plasma Devices

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Abstract

A general law is given for sputtering coefficients as a function of the energy of hydrogen and helium isotope ions incident on metallic and graphite walls and limiters. The average over a Maxwellian spectrum is performed analytically.

1. Introduction

Conceptual design studies of fusion reactor performance, such as the INTOR project, are being undertaken by many nations. A recent review paper by Hershman and Sigmar (1981) gives full details of the effect of impurities in plasmas; another by Ashby and Hughes (1981) combines the evaluation of radiation loss for impurities (Post *et al.* 1977) with transport codes to conclude that in INTOR the temperature radial profile will collapse inwards from the wall. Post *et al.* claimed that the plasma temperature near the wall would be about 200 eV, a temperature at which impurities, particularly from heavy metals, have quite large radiation losses. It is not clear which wall reflective properties were considered to contribute to such losses, but these authors pointed out that the main source of impurities which has considerable power rate coefficients is sputtering from the walls and limiters.

At the AAEC Research Establishment there is insufficient effort to carry out extensive compilations of sputtering coefficients for the hydrogen and helium isotopes, but such a compilation was carried out by Thomas *et al.* (1979). At about the same time, McCracken and Stott (1979) reviewed the semi-empirical theory of sputtering, but their use of the spectral law, developed by Bohdansky, and scaling coefficients did not lead to a particularly good fit of the data and no maximum was predicted in the spectral curve, which occurs in almost all of the data around 1 keV. We have used all available data from Thomas *et al.* to fit the spectrum and to discover the appropriate scaling rules.

2. Semi-empirical Laws

We have chosen the evaluations by Thomas *et al.* to fit the elements Be, C, Ti, Fe, Co, Ni, Cu, Nb, Mo, Ag, Ta, W, Au and U to the rational function

$$S(E) = A(m_1, m_2)\{(E-E_{\mathrm{T}})/(E+B)^2\}, \tag{1}$$

where $E \geqslant E_T$, $S(E)$ is the sputtering coefficient for the incident ion beam energy E, and

$$E_T = E_S/\{\gamma(1-\gamma)\}, \qquad \gamma = 4m_1 m_2/(m_1+m_2)^2; \tag{2a, b}$$

m_1 and m_2 are the atomic masses of the elements in the wall and incident beam respectively and $A(m_1, m_2)$ is the scaling coefficient. The threshold energy E_T can be obtained directly from the sublimation energy of the wall material, defined as E_S (eV), which, in turn, can be obtained from the relation

$$E_S = 0\cdot0435 L_H, \tag{3}$$

where L_H is the latent heat of sublimation (Smithells 1976). If the latent heat is not tabulated, one can use the rough approximations

$$E_S \approx 2\cdot8\times10^{-3} M_p \quad \text{or} \quad 1\cdot48\times10^{-3} B_p, \tag{4}$$

where M_p is the melting point and B_p is the boiling point in K. We have used the second correlation for graphite and silicon only.

It was not possible to find sufficient data to check whether E_T in equation (2a) is the experimental threshold, so we have assumed the theoretical value and computed the constants A and B from the fits to the equation

$$\{(E-E_T)/S(E)\}^{\frac{1}{2}} = a_0 + a_1 E, \tag{5}$$

in which $A = 1/a_1^2$ and $B = a_0/a_1$. The elements used were Be, C, Ti, Fe, Co, Ni, Cu, Nb, Mo, W, Au and U. The maximum of the spectrum occurs when

$$E_{max} = B + 2E_T \tag{6}$$

and the width is so broad that the fits are very insensitive to B. We observed the correlation

$$\bar{E}_{max} = b_0 + b_1 Z_1^{\frac{1}{2}} \tag{7}$$

for Ti, Fe, Ni, Mo, W and Au, where Z_1 is the atomic number of the element in the wall and, with an error weighting of 5%, obtained the values

$$b_0 = -2\cdot5429 \text{ keV and } b_1 = 0\cdot7879 \text{ keV}.$$

We could just as well have found a rough correlation of $\bar{E}_{max}$ with m_1 but, for interpolation purposes, equation (7) suffices.

We note that the scaling factor $A(m_1, m_2)$ in equation (1) can be well approximated by the law

$$A(m_1, m_2) = A(m_1, 1)\exp\{\bar{c}(m_2-1)\}, \tag{8}$$

where $\bar{c}$ is an average value of m_1 and m_2. For this average, we used the data from Thomas *et al.* (1979) for Ti, Fe, Ni, Mo and Au to find

$$\bar{c} = 1\cdot0. \tag{9}$$

Table 1. Experimentally fitted data

Element	m_2	E_S (eV)	E_T (keV)	γ	$A(m_1, m_2)$	$B(Z_1)$ (keV)
^{4}Be	1	3·44	$1\cdot490\times10^{-2}$	$3\cdot619\times10^{-1}$	$4\cdot335\times10^{-1}$	6·150
	2	3·44	$1\cdot430\times10^{-2}$	$5\cdot972\times10^{-1}$	$7\cdot050\times10^{-2}$	$2\cdot025\times10^{-1}$
	4	3·44	$2\cdot726\times10^{-2}$	$8\cdot518\times10^{-1}$	$5\cdot048\times10^{-1}$	$1\cdot750\times10^{-1}$
^{6}C	1	7·42	$3\cdot635\times10^{-2}$	$2\cdot857\times10^{-1}$	$1\cdot672\times10^{-2}$	$4\cdot360\times10^{-1}$
	2	7·42	$2\cdot968\times10^{-2}$	$4\cdot919\times10^{-1}$	$3\cdot373\times10^{-2}$	$3\cdot209\times10^{-1}$
	4	7·42	$3\cdot956\times10^{-2}$	$7\cdot499\times10^{-1}$	$6\cdot868\times10^{-1}$	1·585
^{22}Ti	1	4·88	$6\cdot576\times10^{-2}$	$8\cdot073\times10^{-2}$	$1\cdot703\times10^{-2}$	$9\cdot681\times10^{-1}$
	2	4·88	$3\cdot728\times10^{-2}$	$1\cdot549\times10^{-1}$	$4\cdot275\times10^{-2}$	1·009
	3	4·88	$2\cdot813\times10^{-2}$	$2\cdot234\times10^{-1}$	$1\cdot209\times10^{-1}$	1·268
	4	4·88	$2\cdot396\times10^{-2}$	$2\cdot847\times10^{-1}$	$3\cdot395\times10^{-1}$	1·024
^{26}Fe	1	4·14	$6\cdot507\times10^{-2}$	$6\cdot829\times10^{-2}$	$5\cdot223\times10^{-2}$	1·278
	2	4·14	$3\cdot617\times10^{-2}$	$1\cdot319\times10^{-1}$	$1\cdot224\times10^{-1}$	1·056
	3	4·14	$2\cdot676\times10^{-2}$	$1\cdot913\times10^{-1}$	$2\cdot497\times10^{-1}$	1·128
	4	4·14	$2\cdot237\times10^{-2}$	$2\cdot452\times10^{-1}$	1·071	1·751
^{27}Co	1	4·42	$7\cdot158\times10^{-2}$	$6\cdot612\times10^{-2}$	$1\cdot207\times10^{-1}$	3·056
	2	4·42	$3\cdot965\times10^{-2}$	$1\cdot278\times10^{-1}$	$2\cdot807\times10^{-1}$	2·192
	4	4·42	$2\cdot436\times10^{-2}$	$2\cdot382\times10^{-1}$	5·955	4·562
^{28}Ni	1	4·46	$7\cdot197\times10^{-2}$	$6\cdot638\times10^{-2}$	$9\cdot769\times10^{-2}$	1·513
	2	4·46	$3\cdot988\times10^{-2}$	$1\cdot283\times10^{-1}$	$2\cdot430\times10^{-1}$	1·365
	3	4·46	$2\cdot942\times10^{-2}$	$1\cdot863\times10^{-1}$	$7\cdot519\times10^{-1}$	1·797
	4	4·46	$2\cdot452\times10^{-2}$	$2\cdot390\times10^{-1}$	1·972	2·004
^{29}Cu	1	3·55	$6\cdot153\times10^{-2}$	$6\cdot147\times10^{-2}$	$1\cdot849\times10^{-1}$	$6\cdot632\times10^{-1}$
	2	3·55	$3\cdot383\times10^{-2}$	$1\cdot191\times10^{-1}$	$5\cdot394\times10^{-1}$	1·632
	4	3·55	$2\cdot049\times10^{-2}$	$2\cdot230\times10^{-1}$	5·167	3·298
^{41}Nb	1	7·50	$1\cdot844\times10^{-1}$	$4\cdot246\times10^{-2}$	$3\cdot266\times10^{-2}$	3·110
	2	7·50	$9\cdot846\times10^{-2}$	$8\cdot307\times10^{-2}$	$8\cdot207\times10^{-2}$	3·252
	4	7·50	$5\cdot626\times10^{-2}$	$1\cdot584\times10^{-1}$	3·152	8·552
^{42}Mo	1	6·90	$1\cdot749\times10^{-1}$	$4\cdot115\times10^{-2}$	$3\cdot180\times10^{-2}$	3·877
	2	6·90	$9\cdot316\times10^{-2}$	$8\cdot056\times10^{-2}$	$6\cdot546\times10^{-2}$	2·157
	3	6·90	$6\cdot607\times10^{-2}$	$1\cdot185\times10^{-1}$	$1\cdot432\times10^{-1}$	2·136
	3	6·90	$6\cdot607\times10^{-2}$	$1\cdot185\times10^{-1}$	$3\cdot288\times10^{-1}$	2·355
	4	6·90	$5\cdot302\times10^{-2}$	$1\cdot538\times10^{-1}$	$5\cdot575\times10^{-1}$	2·273
^{74}W	1	8·81	$4\cdot152\times10^{-1}$	$2\cdot169\times10^{-2}$	$4\cdot012\times10^{-3}$	2·534
	2	8·81	$2\cdot147\times10^{-1}$	$4\cdot288\times10^{-2}$	$1\cdot793\times10^{-2}$	3·219
	4	8·81	$1\cdot152\times10^{-1}$	$8\cdot341\times10^{-2}$	$7\cdot737\times10^{-1}$	5·134
^{79}Au	1	3·94	$1\cdot985\times10^{-1}$	$2\cdot026\times10^{-2}$	$3\cdot162\times10^{-1}$	5·042
	2	3·94	$1\cdot024\times10^{-1}$	$4\cdot008\times10^{-2}$	$7\cdot477\times10^{-1}$	4·189
	3	3·94	$7\cdot034\times10^{-2}$	$5\cdot956\times10^{-2}$	1·252	3·884
	3	3·94	$7\cdot034\times10^{-2}$	$5\cdot956\times10^{-2}$	2·570	4·342
	4	3·94	$5\cdot474\times10^{-2}$	$7\cdot808\times10^{-2}$	2·761	3·197
^{92}U	1	4·76	$2\cdot883\times10^{-1}$	$1\cdot679\times10^{-2}$	$3\cdot627\times10^{-2}$	18·16
	4	4·76	$7\cdot826\times10^{-2}$	$6\cdot506\times10^{-2}$	1·519	22·39

Thomas *et al.* reported old experimental values for $S(E)$ by Kenknight and Wehner (1964) for eighteen elements at the energies of 2·33 and 3·5 keV for incident H^+ ions. They warned that the quoted error of 3% was unrealistic and differed from more recent measurements by factors of two. However, their graphs show quite definite regions,

$$\text{(i) } 22 \leqslant Z_1 \leqslant 29, \qquad \text{(ii) } 41 \leqslant Z_1 \leqslant 47, \qquad \text{(iii) } 74 < Z_1 \leqslant 79, \tag{10}$$

in which the scaling law

$$A(m_1, 1) = \exp(c_0 + c_1 m_1) \tag{11}$$

holds. For a least-squares fit over region (i) for five atoms, we obtained

$$c_{01} = -11{\cdot}393, \qquad c_{11} = 0{\cdot}15362. \tag{12}$$

Assuming the same slope in region (ii), we found, from the accurate Mo data, that

$$c_{02} = -18{\cdot}187, \qquad c_{12} = c_{11}; \tag{13}$$

Table 2. Predicted values of A and B

Element	m_2	E_S (eV)	E_T (keV)	γ	$A(m_1, m_2)$	$B(Z_1)$ (keV)
^{13}Al	1	4·09	$3{\cdot}421\times10^{-2}$	$1{\cdot}388\times10^{-1}$	$4{\cdot}503\times10^{-2}$	$2{\cdot}294\times10^{-1}$
	2	4·09	$2{\cdot}134\times10^{-2}$	$2{\cdot}585\times10^{-1}$	$1{\cdot}257\times10^{-1}$	$2{\cdot}551\times10^{-1}$
	3	4·09	$1{\cdot}770\times10^{-2}$	$3{\cdot}624\times10^{-1}$	$3{\cdot}461\times10^{-1}$	$2{\cdot}624\times10^{-1}$
	4	4·09	$1{\cdot}653\times10^{-2}$	$4{\cdot}500\times10^{-1}$	$9{\cdot}225\times10^{-1}$	$2{\cdot}648\times10^{-1}$
^{14}Si	1	4·68	$4{\cdot}039\times10^{-2}$	$1{\cdot}338\times10^{-1}$	$8{\cdot}435\times10^{-4}$	$3{\cdot}243\times10^{-1}$
	2	4·68	$2{\cdot}498\times10^{-2}$	$2{\cdot}497\times10^{-1}$	$2{\cdot}325\times10^{-3}$	$3{\cdot}551\times10^{-1}$
	3	4·68	$2{\cdot}055\times10^{-2}$	$3{\cdot}510\times10^{-1}$	$6{\cdot}380\times10^{-3}$	$3{\cdot}640\times10^{-1}$
	4	4·68	$1{\cdot}902\times10^{-2}$	$4{\cdot}367\times10^{-1}$	$1{\cdot}699\times10^{-2}$	$3{\cdot}670\times10^{-1}$
^{21}Sc	1	3·91	$4{\cdot}986\times10^{-2}$	$8{\cdot}578\times10^{-2}$	$1{\cdot}126\times10^{-2}$	$9{\cdot}679\times10^{-1}$
	2	3·91	$2{\cdot}850\times10^{-2}$	$1{\cdot}642\times10^{-1}$	$3{\cdot}103\times10^{-2}$	1·011
	3	3·91	$2{\cdot}167\times10^{-2}$	$2{\cdot}362\times10^{-1}$	$8{\cdot}515\times10^{-2}$	1·024
	4	3·91	$1{\cdot}861\times10^{-2}$	$3{\cdot}003\times10^{-1}$	$2{\cdot}267\times10^{-1}$	1·030
^{23}V	1	4·88	$6{\cdot}941\times10^{-2}$	$7{\cdot}610\times10^{-2}$	$5{\cdot}044\times10^{-2}$	1·097
	2	4·88	$3{\cdot}906\times10^{-2}$	$1{\cdot}463\times10^{-1}$	$1{\cdot}418\times10^{-1}$	1·158
	3	4·88	$2{\cdot}926\times10^{-2}$	$2{\cdot}116\times10^{-1}$	$3{\cdot}917\times10^{-1}$	1·177
	4	4·88	$2{\cdot}475\times10^{-2}$	$2{\cdot}702\times10^{-1}$	1·046	1·186
^{24}Cr	1	5·36	$7{\cdot}763\times10^{-2}$	$7{\cdot}461\times10^{-2}$	$3{\cdot}319\times10^{-2}$	1·162
	2	5·36	$4{\cdot}358\times10^{-2}$	$1{\cdot}436\times10^{-1}$	$9{\cdot}151\times10^{-2}$	1·230
	3	5·36	$3{\cdot}257\times10^{-2}$	$2{\cdot}077\times10^{-1}$	$2{\cdot}511\times10^{-1}$	1·252
	4	5·36	$2{\cdot}749\times10^{-2}$	$2{\cdot}655\times10^{-1}$	$6{\cdot}684\times10^{-1}$	1·262
^{30}Zn	1	1·37	$2{\cdot}437\times10^{-2}$	$5{\cdot}980\times10^{-2}$	$2{\cdot}593\times10^{-1}$	1·724
	2	1·37	$1{\cdot}336\times10^{-2}$	$1{\cdot}160\times10^{-1}$	$7{\cdot}150\times10^{-1}$	1·746
	3	1·37	$9{\cdot}756\times10^{-3}$	$1{\cdot}690\times10^{-1}$	1·962	1·753
	4	1·37	$8{\cdot}051\times10^{-3}$	$2{\cdot}174\times10^{-1}$	5·222	1·756
^{40}Zr	1	6·36	$1{\cdot}538\times10^{-1}$	$4{\cdot}323\times10^{-2}$	$4{\cdot}144\times10^{-2}$	2·133
	2	6·36	$8{\cdot}217\times10^{-2}$	$8{\cdot}454\times10^{-2}$	$1{\cdot}177\times10^{-1}$	2·276
	3	6·36	$5{\cdot}847\times10^{-2}$	$1{\cdot}242\times10^{-1}$	$3{\cdot}262\times10^{-1}$	2·323
	4	6·36	$4{\cdot}707\times10^{-2}$	$1{\cdot}611\times10^{-1}$	$8{\cdot}724\times10^{-1}$	2·346
^{45}Rh	1	5·78	$1{\cdot}565\times10^{-1}$	$3{\cdot}842\times10^{-2}$	$9{\cdot}248\times10^{-2}$	2·429
	2	5·78	$8{\cdot}300\times10^{-2}$	$7{\cdot}531\times10^{-2}$	$2{\cdot}550\times10^{-1}$	2·576
	3	5·78	$5{\cdot}861\times10^{-2}$	$1{\cdot}109\times10^{-1}$	$6{\cdot}996\times10^{-1}$	2·625
	4	5·78	$4{\cdot}685\times10^{-2}$	$1{\cdot}442\times10^{-1}$	1·862	2·649
^{47}Ag	1	1·78	$5{\cdot}037\times10^{-2}$	$3{\cdot}668\times10^{-2}$	$3{\cdot}122\times10^{-1}$	2·758
	2	1·78	$2{\cdot}665\times10^{-2}$	$7{\cdot}197\times10^{-2}$	$8{\cdot}679\times10^{-1}$	2·805
	4	1·78	$1{\cdot}496\times10^{-2}$	$1{\cdot}380\times10^{-1}$	6·365	2·829
^{73}Ta	1	8·13	$3{\cdot}773\times10^{-1}$	$2{\cdot}203\times10^{-2}$	$1{\cdot}778\times10^{-2}$	3·434
	2	8·13	$1{\cdot}952\times10^{-1}$	$4{\cdot}355\times10^{-2}$	$5{\cdot}102\times10^{-2}$	3·798
	4	8·13	$1{\cdot}049\times10^{-1}$	$8{\cdot}469\times10^{-2}$	$3{\cdot}800\times10^{-1}$	3·979

similarly, using the Au information,

$$c_{03} = -31\cdot409, \qquad c_{13} = c_{11}. \tag{14}$$

3. Details of Data

As was the case with the ADL-1 atomic data library (Clancy *et al.* 1981), preparation of the sputtering coefficient data library was based on the use of all experimental information, resorting to the constants in the fitted law (1) only for interpolation and extrapolation when experimental data were unavailable. The best fits for E_S, E_T, γ, A and B are displayed in Table 1. The predicted values of A and B are shown in Table 2 for Al, Si, Sc, V, Cr, Zn, Zr, Rh, Ag and Ta. The elements Al, Zr and Ta can be normalized to the measured value of $A(m_1, 1)$.

The compilation by Thomas *et al.* gives tables and plots for the sputtering of incident H^+, D^+, T^+, He_3^+ and He_4^+ ion beams from the elements Be, C, Ti, Fe, Co, Ni, Cu, Nb, Mo, Ag, Ta, W, Au and U, although the information is sometimes very scanty indeed. The fitted spectra of some of these elements are given in Fig. 1 on a log–log scale. It is noted that the deviation from the experimental values is the largest at very low energies; we believe that this is because $S(E)$ is very small in this region and that the predicted values of E_T could be in error. The data here are very sensitive to the value of E_T.

McCracken and Stott (1979) also gave a general curve for $\bar{S}(T)$, the average value of $S(E)$ over a Maxwellian ion energy distribution, which is appropriate for plasmas. Because of their use of the Bohdansky spectral law, the necessary integral cannot be evaluated analytically. In contrast, the form of equation (1) can be averaged analytically.

4. Maxwellian Averaged Sputtering Coefficients

The integral which has to be calculated is

$$\bar{S}(T) = 2\pi^{-\frac{1}{2}}T^{-3/2}\int_{E_T}^{\infty} \mathrm{d}E\, S(E)\, E^{\frac{1}{2}}\exp(-E/T), \tag{15}$$

where T is the temperature of the plasma edge in keV. This can be written

$$\begin{aligned}\bar{S}(T) &= 2\pi^{-\frac{1}{2}}T^{-3/2}\left(\int_0^{\infty} \mathrm{d}E\, S(E)\, E^{\frac{1}{2}}\exp(-E/T) - \int_0^{E_T} \mathrm{d}E\, S(E)\, E^{\frac{1}{2}}\exp(-E/T)\right)\\ &= I_1 - I_2 .\end{aligned} \tag{16}$$

Substituting equation (1) into (16), we find that (Gradshteyn and Ryzhik 1965)

$$\int_0^{\infty} \mathrm{d}E\, S(E)\, E^{\frac{1}{2}}\exp(-E/T) = A(I_1^1 - E_T I_2^1), \tag{17}$$

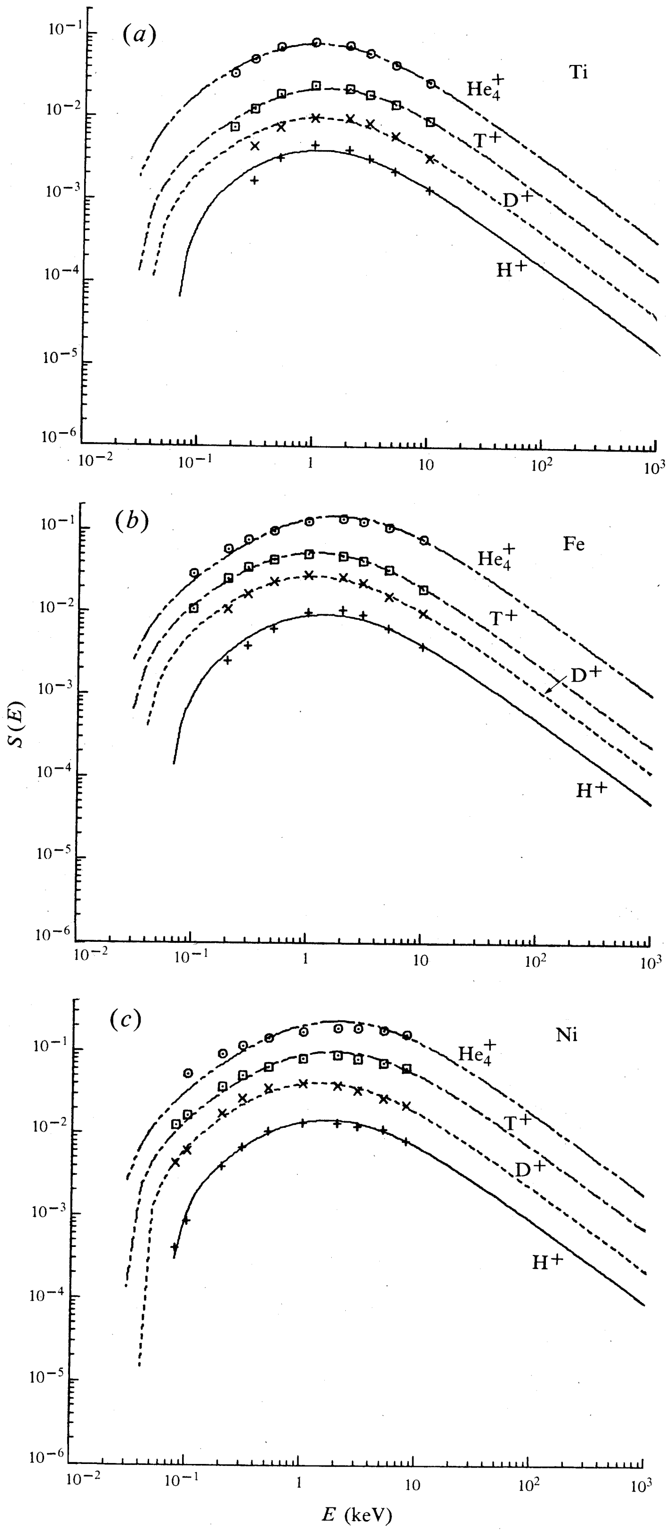
where

$$I_1^1 = 4\Gamma\tfrac{5}{2}\mu^{-\frac{5}{4}}\exp(\tfrac{1}{4}z^2)D_{-4}(z), \tag{18}$$

$$I_2^1 = 2^{3/2}\Gamma\tfrac{3}{2}B^{-\frac{3}{4}}\exp(\tfrac{1}{4}z^2)D_{-3}(z), \tag{19}$$

and A is defined by equation (8). In these equations

$$\mu = 1/T, \qquad z = (2B/T)^{\frac{1}{2}}, \tag{20}$$



Figs 1*a-c*. [*See caption on opposite page.*]

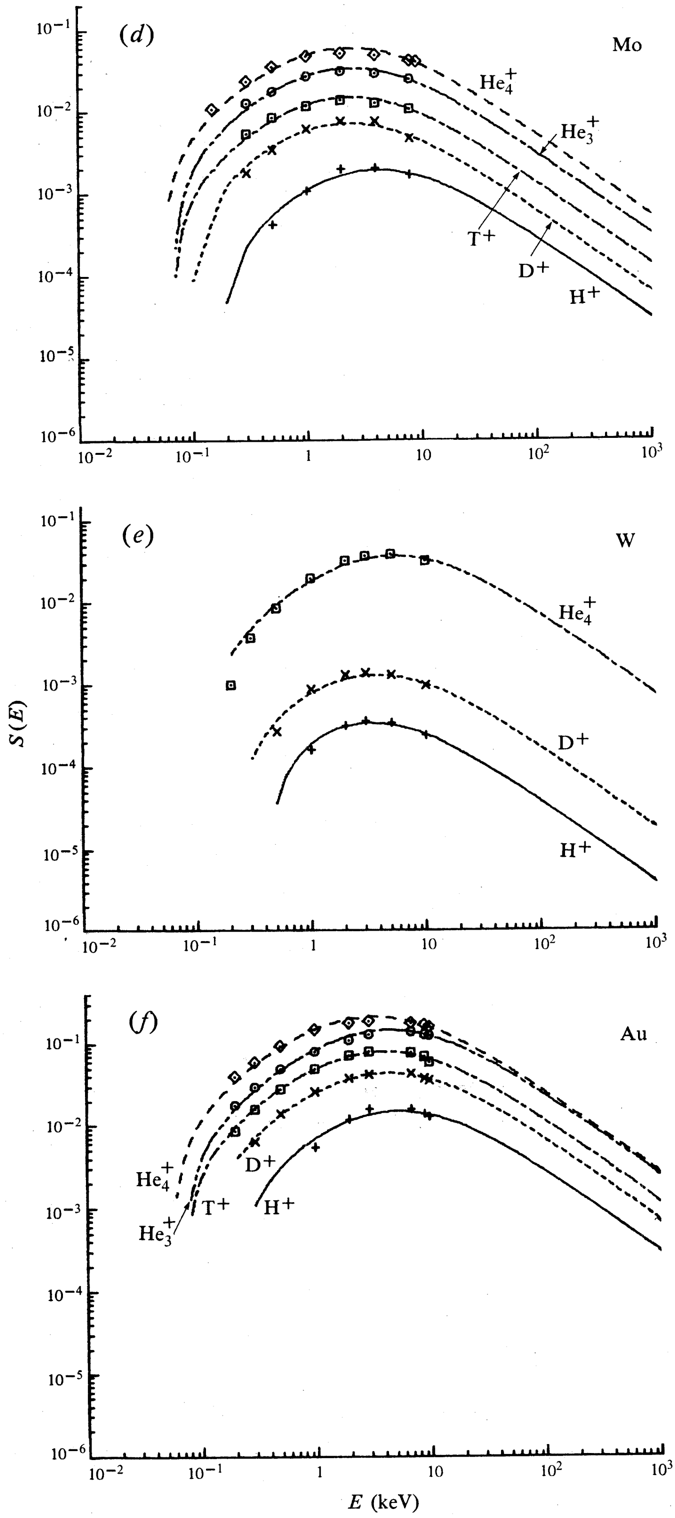


Fig. 1. Calculated curves and experimental points showing sputtering coefficients as a function of energy for the sputtering of incident H^+, D^+, T^+, He_3^+ and He_4^+ ion beams from various elements.

and $D_\nu(z)$ is the parabolic cylinder function. This function is tabulated by Abramowitz and Stegun (1965) for $0 \leqslant z \leqslant 5$, and can be computed from the recurrence relation of Erdélyi *et al.* (1953)

$$D_{\nu-1}(z) = \nu^{-1}\{zD_\nu(z) - D_{\nu+1}(z)\}. \tag{21}$$

For the first two cases

$$D_{-1}(z) = (\tfrac{1}{2}\pi)^{\frac{1}{2}}\exp(\tfrac{1}{4}z^2)\,\mathrm{erfc}(\sqrt{\tfrac{1}{2}}\,z), \tag{22}$$

$$D_{-2}(z) = zD_{-1}(z) - \exp(\tfrac{1}{4}z^2), \tag{23}$$

where

$$\mathrm{erfc}(x) = 2\pi^{-\frac{1}{2}}\int_x^\infty \exp(-t^2)\,\mathrm{d}t.$$

For very low temperatures, the asymptotic series

$$\exp(\tfrac{1}{4}z^2)\,D_\nu(z) = z^\nu\left(1 - \frac{\nu(\nu-1)}{2z^2} + \frac{\nu(\nu-1)(\nu-2)(\nu-3)}{2!(2z^2)^2}\right) \tag{24}$$

can be used, and higher terms can be found in equation (21).

The second integral in equation (16) can be approximated very well by expanding both the exponential term and the denominator into Taylor series and integrating term-by-term. From this we get

$$I_2 \approx (A/B^2)\sum_{n=0}^{\infty}\{(-1)^n/n!\}E_{\mathrm{T}}^{5/2}(E_{\mathrm{T}}/T)^n[\{1+(2E_{\mathrm{T}}/B)\}(n+\tfrac{5}{2})^{-1} - (n+\tfrac{3}{2})^{-1} - (2E_{\mathrm{T}}/B)(n+\tfrac{7}{2})^{-1}], \tag{25}$$

with a maximum error of about 1% close to threshold.

5. Discussion

It will be noticed that in Fig. 1 the first few experimental points sometimes fall below the calculated threshold, in the low temperature region; various effects can account for this. The most probable explanation is that the thermal spread of the local bonding in the region of the incident ion impact smears out the values of the sublimation energy, so that sub-threshold sputtering becomes possible. Unfortunately, none of the data reported by Thomas *et al.* (1979) contain point-by-point errors, hence we could not perform a systematic error analysis on the data fits to equation (1).

McCracken and Stott (1979) found an appreciable upward shift in their Maxwellian average maximum temperature. This is because the Bohdansky law predicts a continuous rise in the spectrum, and the contribution from the high temperature region is much too large. We found a much smaller upward shift.

A full library of Maxwellian averages for all of the elements analysed by Thomas *et al.* is available at the AAEC. It is proposed that this information be included in the ADL-1 atomic data library for computations of plasma behaviour in conceptual fusion reactor design studies. A zero-dimensional code, SCORCH, has been written to enable benchmark calculations to be carried out as a check on the data from the plasma devices now in use.

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