Distribution Categories:
Magnetic Fusion Energy (UC-20)
MFE—Theoretical Plasma Physics
(UC-20g)

ANL/FPP/TM-171

ANL/FPP/TM--171

DE83 012305

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

**CHARGE STATE OF SPUTTERED IMPURITY IONS NEAR
A LIMITER OR DIVERTOR IN A TOKAMAK**

by

C. D. Boley, J. N. Brooks, and Y.-K. Kim

Fusion Power Program

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

March 1983

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	1
INTRODUCTION	3
MODEL	3
RESULTS	8
APPENDIX A: Ionization Cross Sections of Tungsten Ions	11
APPENDIX B: Kinematics	13
REFERENCES	15

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1	Model geometry.	4
2	Maxwellian averaged ionization rate coefficients for tungsten.	6

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1	Final Charge State Z_f and Final Kinetic Energy E_f	8
A-1	Cross-Section Constants for Tungsten Ions to be Used with Eq. (A-1)	12

CHARGE STATE OF SPUTTERED IMPURITY IONS NEAR A LIMITER OR DIVERTOR IN A TOKAMAK

C. D. Boley, J. N. Brooks, and Y.-K. Kim

**Fusion Power Program
Argonne National Laboratory
Argonne, Illinois 60439**

ABSTRACT

Many impurity atoms sputtered from a limiter or divertor plate are ionized in the scrapeoff zone and return to the sputtering surface because of friction with incoming plasma ions. The final charge state attained by such impurities has been calculated for a variety of plasma edge conditions. The surface materials considered are tungsten, beryllium, beryllium oxide, and carbon. Estimates of the successive ionization cross sections for tungsten are developed. In all cases examined, returning impurity ions are found to be multiply ionized. This implies a significant energy gain in the sheath region, with important implications for self-sputtering of redeposited surface material.

INTRODUCTION

Limiters and divertors have been proposed as impurity control devices for future tokamak fusion reactors. A critical issue with these devices is the surface erosion caused by sputtering. Typically, atoms sputtered from the impurity control system will be ionized within the scrapeoff region and will then flow back to the surface, where they can stick and/or self-sputter. This redeposition process has been found to be critical in determining the lifetime of these devices and the impurity content in the plasma.⁽¹⁾ The charge state of redeposited impurity ions is important because it determines the energy acquired in the sheath region, thus affecting the self-sputtering coefficients. Also of concern is the energy acquired, through collisions, prior to the sheath. The charge state is important for all surface materials but is particularly so for high-Z materials such as tungsten or tantalum, for which the final impact energy of returning ions must be limited to about 700 eV, in order to hold the self-sputtering coefficient to values less than unity. If these materials are employed, therefore, the charge state has a direct bearing on the maximum permissible plasma edge temperature.

The charge state of sputtered atoms, ionized in the scrape-off zone, was computed for a variety of possible plasma edge conditions, using models for sputtering, ionization, and momentum transfer with the incoming plasma. The materials considered were tungsten (typical of high-Z materials) and the low-Z coatings of beryllium, beryllium oxide, and carbon. It was found that sputtered atoms of all these materials become multiply charged before returning to the surface. This has important implications for sputtering calculations.

MODEL

In the model used here, a newly ionized impurity particle acquires momentum from the incoming D-T ions and from the possible presence of a pre-sheath electric field. The resulting particle trajectory is followed, along with the solution of a series of rate equations giving the instantaneous charge state. When the impurity ion hits the surface its final charge state is noted. An average over many trajectories is taken. Figure 1 shows the model geometry. For most reactor designs the magnetic field intersects the

Fig. 1. Model geometry (top view). The neutral is sputtered into a polar angle θ with respect to the normal from the plate, and the magnetic field intercepts the plate with a polar angle θ_B .

impurity control surface at a very shallow angle (≤ 5 deg), in order to spread the heat load. The sheath region is small compared to the distance traveled by the sputtered impurities.

In the sputtering event under consideration, a neutral is emitted from the surface into a given angle, and travels a given distance before ionization. After ionization, which is assumed to involve negligible momentum transfer, the ion executes a spiral motion along the local magnetic field line. The initial parallel velocity can be in either direction, depending on the angle of emission. The model for the parallel motion is

$$\frac{dv_{\parallel}(t)}{dt} = -v(t)[v_{\parallel}(t) - v_{DT}] + \frac{Z(t)e}{m} E_{\parallel} ,$$

where $\bar{Z}(t)$ is the instantaneous mean charge state, m is the mass of the impurity, $v_{DT} = (T_e/m_{DT})^{1/2}$, ν is the Braginskii 90-deg collision frequency,

$$\nu(t) = \frac{4(2\pi)^{1/2} n_{DT} e^4 \ln \Lambda}{3(4\pi\epsilon_0)^2 T_i^{3/2}} \left[\frac{m_{DT}}{m(m + m_{DT})} \right]^{1/2} \bar{Z}^2(t) ,$$

and $\bar{Z}^2(t)$ is the mean squared charge state. The D-T ions stream from the field line toward the plate, and the resulting friction tends to slow down an impurity initially moving away from the plate. Perpendicular equilibration has been ignored, since in this problem it occurs much more slowly than parallel equilibration.

The time-dependent distribution of charge states is calculated from the coronal rate equations,

$$\frac{dn_i}{dt} = -\nu_i n_i + \nu_{i-1} n_{i-1} , \quad (i \geq 1, \nu_0 = 0) ,$$

where n_i is the population of the i -th ionization state and ν_i is the rate coefficient for ionization from charge state i to charge state $(i + 1)$. For the temperatures of interest, ionization occurs almost exclusively via electron impact, and so one has

$$\begin{aligned} \nu_i &= n_e \langle \sigma_i v \rangle \\ &= n_e \left(\frac{8}{\pi m_e T_e^3} \right)^{1/2} \int_0^\infty dE E e^{-E/T_e} \sigma_i(E) , \end{aligned}$$

where the indicated average over an electron distribution function with temperature T_e has been taken, and E is the electron impact energy. Recombination is unimportant at the relatively low charge states encountered here. For beryllium, carbon, and oxygen, the ionization cross sections were taken from Ref. 2. For tungsten, cross sections described in Appendix A were employed. The dependence on T_e of the first several Maxwellian-averaged tungsten cross sections is shown in Fig. 2.

Fig. 2. Maxwellian averaged ionization rate coefficients for tungsten. The cross sections were calculated according to the prescription in Appendix A.

At any time the mean charge state and the mean squared charge state are given by

$$\bar{z} = \sum_i z_i n_i / \sum_i n_i, \quad \overline{z^2} = \sum_i z_i^2 n_i / \sum_i n_i.$$

In practice, there is negligible difference between $(\bar{z})^2$ and $\overline{z^2}$.

The instantaneous charge state affects not only the parallel friction and the coupling to the electric field but also the Larmor radius, since as $\bar{z}$ increases, the spiral becomes more tightly wound. For the lighter elements, the Larmor frequency is sufficiently high so that one can consider the trajectory as defining a cylinder of gradually decreasing radius. For heavier elements such as tungsten the corkscrew motion must be followed in detail. Some details of the kinematics are noted in Appendix B.

A computer code has been written to solve for the motion of the impurity. The code records the charge state and kinetic energy at the moment of impact with the surface, and then takes an average over sputtering energies, solid angles of emission, and ionization distances. In the examples considered here, the sputtering energies were distributed according to a random collision cascade model³

$$F(E) \sim \frac{E}{(E + U_0)^3},$$

where U_0 is the surface binding energy. Ten energies were sampled. The solid angles, which were weighted by the cosine with respect to the normal, were taken from the 38 discrete-ordinates package commonly used in neutronics calculations. The average over ionization distances was accomplished by a five-point Gauss-Laguerre integration scheme. In the case of the lighter elements some trajectories involved relatively long excursions along the field line, on the order of tens of meters. A cutoff distance of 10 m was defined, beyond which a trajectory was considered lost to the plasma and was not included in the averages.

RESULTS

Table 1 shows the final charge state Z_f and kinetic energy K_f for several elements and for a selection of edge conditions. These edge conditions range over "low" (20 eV), "medium" (100 eV), and "high" (700 eV) edge temperature

Table 1. Final Charge State Z_f and Final Kinetic Energy E_f
(Prior to the Sheath) Attained by Sputtered Atoms,
for Various Plasma Edge Conditions

For comparison, the coronal-equilibrium value of the charge state (from Ref. 5) at the given electron temperature is listed as Z_{cor} . In all cases, $B_t = 5$ T, $B_p = 0.5$ T, and the angle between B_p and the surface is 15 deg. A dash signifies that all sputtered ions were lost to the plasma.

T_e (eV)	n_e (m^{-3})	Z_{cor}	$E_{ } = 100 \text{ V/m}$		$E_{ } = 0$		$E_{ } = -100 \text{ V/m}$	
			Z_f	K_f (eV)	Z_f	K_f (eV)	Z_f	K_f (eV)
<u>Beryllium ($U_0 = 3.4 \text{ eV}$)</u>								
20	2.5×10^{19}	2.24	1.74	47.1	1.79	33.2	1.85	22.0
100	9.26×10^{19}	3.98	1.92	33.0	1.95	26.8	2.01	20.8
700	5.0×10^{18}	4.	1.90	195.9	2.76	22.4	----	----
<u>Beryllium ($U_0 = 6.1 \text{ eV}$)</u>								
100	9.26×10^{19}	3.98	1.94	50.0	1.98	41.7	2.03	33.8
700	5.0×10^{18}	4.	1.96	264.3	2.82	37.0	----	----
<u>Carbon ($U_0 = 7.4 \text{ eV}$)</u>								
100	9.26×10^{19}	5.29	2.66	68.2	2.74	59.3	2.84	50.6
700	5.0×10^{18}	6.	2.56	261.4	3.61	44.6	----	----
<u>Oxygen ($U_0 = 6.1 \text{ eV}$)</u>								
100	9.26×10^{19}	6.02	3.05	80.2	3.14	68.7	3.26	57.5
700	5.0×10^{18}	8.	3.06	301.2	4.52	45.0	----	----
<u>Tungsten ($U_0 = 11.1 \text{ eV}$)</u>								
20	2.5×10^{19}	2.42 ^a	2.88	96.5	2.91	90.7	2.95	84.9
50	2.5×10^{19}	6.06 ^a	3.95	92.4	4.03	85.4	4.12	78.4
50	5.0×10^{19}	6.06 ^a	3.83	77.3	3.85	74.9	3.89	72.4

^aEstimated by linear interpolation between the value at $T_e = 80$ eV (lowest temperature available in Ref. 5) and the vanishing value at $T_e = 0$.

regions currently thought to be obtainable in a tokamak reactor (see, for example, Ref. 4). Since the value of the parallel electric field is not well established, the values $E_{\parallel} = 0$ and $E_{\parallel} = \pm 100$ v/m were surveyed. Two binding energies were considered for beryllium, corresponding to pure beryllium ($U_0 = 3.4$ eV) and beryllium oxide ($U_0 = 6.1$ eV). The following points can be noted:

- (1) As the electric field increases, the final charge state decreases and the final kinetic energy increases, as would be expected.
- (2) The final energy (prior to the sheath) is, in all cases, considerably less than the value $m/m_{DT} (T/2)$ which would be attained for full equilibration of impurities and D-T ions in the parallel direction. Thus the time for sputtered atoms ionized in the scrapeoff zone to return to the surface is short compared to the equilibration time. Nevertheless, all elements became multiply charged, although this charge is about one-half of the coronal equilibrium value at the respective edge temperature.
- (3) For tungsten at 50 eV, as the electron density increases from $2.5 \times 10^{13} \text{ m}^{-3}$ to $5.0 \times 10^{19} \text{ m}^{-3}$, the final charge state is nearly constant. The reason is that the increase in higher ionization frequencies offsets the decrease in the neutral mean free path. While the charge states do vary with edge temperature, this variation is not very large, in the context of other uncertainties related to sputtering, edge physics, etc. Thus, for the purpose of sputtering calculations, one can use typical charge-state values of $Z_f = 2$ for beryllium, $Z_f = 3$ for carbon, $Z_f = 3$ for oxygen, and $Z_f = 3-4$ for tungsten.

To test the sensitivity of the results to the ionization cross sections, some additional runs were made with the cross sections divided by two and other runs were made with the cross sections multiplied by two. The charge states changed only slightly under these conditions, decreasing by less than 10% in the former case and increasing by about the same amount in the latter case. The explanation for this insensitivity is similar to that noted above -- if the cross sections are decreased, the neutral travels further from the plate before being ionized, and so the ion is allowed to travel a longer distance; and vice versa if the cross sections are increased. (Note that scaling the cross sections is not quite equivalent to scaling the density, since the

plasma collision frequency is affected only in the latter case.) The final energy changed more substantially under these variations. When the cross sections were halved, K_f increased by amounts ranging from 10% to 50%, depending on the particular case, and it decreased correspondingly when the cross sections were doubled. This sensitivity, however, is not too important since K_f is always smaller than the energy $3 Z_f T_e$ acquired in the sheath.

The effect of perpendicular diffusion was also considered. This was done by replacing a single incoming particle trajectory by three trajectories spread in the perpendicular direction. These were weighted by a Gaussian distribution based on a diffusion coefficient of $1.0 \text{ m}^2/\text{s}$. The resulting charge states showed only small changes from the no-diffusion cases. This is so for two reasons: (1) the diffusion lengths are fairly small due to the short times involved; and (2) the effect of particles diffusing towards the surface and away from the surface tend to cancel each other.

APPENDIX A

Ionization Cross Sections of Tungsten Ions

No theoretical or experimental estimate of cross sections for the electron-impact ionization of tungsten ions is available in the literature. To provide order of magnitude estimates, cross sections were determined in the following manner.

For convenience, the electron-impact ionization cross section, σ_{ion} , is written as a function of the incident energy E in unit of the lowest ionization potential I , $x = E/I$:

$$\sigma_{ion} = \frac{4\pi a_0^2 R^2}{I^2 x} [A \ln x + B(1 - 1/x) + C \ln x/(1 + x)] , \quad (A-1)$$

where

$$a_0 = 0.529 \text{ \AA}$$

$$R = 13.6 \text{ eV}$$

A, B, C = adjustable constants.

Equation (A-1) has the advantage that σ_{ion} vanishes at the threshold ($x = 1$), and σ_{ion} can be evaluated quickly at any incident energy. Furthermore, Eq. (A-1) reduces to the correct asymptotic form

$$\sigma_{ion} \sim \frac{4\pi a_0^2}{I^2 x} [A \ln x + B] , \quad (A-2)$$

when $x \gg 1$.

To determine the adjustable constants, we used a guideline relating the maximum ionization cross section σ_{max} with the geometrical cross section $\pi \langle r^2 \rangle$ of the valence shell:

$$\sigma_{max} = D \langle r^2 \rangle \pi a , \quad (A-3)$$

where

$$D = \begin{cases} 2/3 & \text{for a closed shell,} \\ 1/2 & \text{for an open shell, and} \\ 1/3 & \text{for one electron outside a closed shell.} \end{cases} \quad (\text{A-4})$$

The values of D listed above reflect experience with smaller ions for which ionization cross sections are known.

The values of I were chosen from experimental and theoretical values. The theoretical values were calculated from relativistic Hartree-Fock wavefunctions with average configurations. The shell sizes, $\langle r^2 \rangle$, were also calculated from the relativistic Hartree-Fock wavefunctions. After the values of I and $\langle r^2 \rangle$ were chosen, the constants A , B , and C in Eq. (A-1) were adjusted to have σ_{ion} reach its maximum, σ_{max} , near $x = 3-4$. The higher the ionicity, the sooner the maximum is reached, i.e., at a smaller value of x .

The values of I , σ_{max} , A , B , and C are listed in Table A-1. The cross sections derived from the constants in Table A-1 should be used with a philosophy that a crude estimate is better than nothing. We do not expect, for instance, our estimate to shed any light on the complicated autoionization of inner-shell excited states near the threshold that could overwhelm the threshold region. Deviations of 200-300% from reality should not be ruled out in using the cross sections presented in Table A-1.

Table A-1. Cross-Section Constants for Tungsten Ions to be Used with Eq. (A-1)

Ion	I (eV)	σ_{max} ($\text{\AA}^2$)	A	B	C
W	7.13	8.1	1.26	4	-8
W^+	14.2	3.3	3.1	3.4	-10
W^{2+}	25.3	2.4	6.5	4	-10
W^{3+}	37.2	1.6	10	3	-10
W^{4+}	50.1	1.4	16	3	-12
W^{5+}	64.0	0.85	16	3	-13
W^{6+}	121.4	1.0	68	6	-40
W^{7+}	139.4	0.72	65	6	-40
W^{8+}	158.0	0.70	80	6	-40
W^{9+}	177.1	0.45	66	5	-40
W^{10+}	208.1	0.78	150	6	-48

APPENDIX B

Kinematics

Consider a neutral atom sputtered with energy E_0 into the solid angle (θ, ϕ) , with θ measured from the vertical and ϕ measured from the line on the plate beneath the incoming magnetic field line [cf. Fig. 1. The magnetic field is taken to intersect the plate from above, and so its solid angle is $(\pi - \theta_B, -\pi)$. Suppose the neutral travels a distance l before ionization. At the point of ionization (a distance $l \cos \theta$ above the plate), define a coordinate system such that the z -axis is parallel to $\vec{B}$, the x -axis lies in the direction of $\hat{n} \times \hat{z}$, with $\hat{n}$ the normal from the plate, and of course $\hat{y} = \hat{z} \times \hat{x}$. Then the gyromotion of the ion takes place in the x - y plane and is given by:

$$\begin{aligned} x(t) &= \frac{v_y(0)}{\Omega} + \frac{1}{\Omega} [v_x(0) \sin \Omega t - v_y(0) \cos \Omega t] \\ y(t) &= -\frac{v_x(0)}{\Omega} + \frac{1}{\Omega} [v_y(0) \sin \Omega t + v_x(0) \cos \Omega t], \end{aligned}$$

with $\Omega = ZeB/m$. (Note that the frequency is here treated as a constant, since it changes negligibly during a gyroperiod.) The first term on the right-hand side gives the location of the gyrocenter. The initial velocity of the ion, which is assumed to be the same as the velocity of the neutral, has the components:

$$\begin{aligned} v_x(0) &= -v_0 \sin \theta \sin \phi, \\ v_y(0) &= v_0 (\cos \theta \cos \theta_B - \sin \theta \sin \theta_B \cos \phi), \\ v_z(0) &= -v_0 (\cos \theta \sin \theta_B + \sin \theta \cos \theta_B \cos \phi), \end{aligned}$$

where $v_0 = (2 E_0/m)^{1/2}$. If $v_z(0) < 0$ the gyrocenter initially moves up the field line, away from the plate.

The distance along the field line from the point of ionization to the plate is $z_0 = l \cos \theta / \sin \theta_B$. Because of the ion's gyromotion, the actual net parallel distance $z(t_0)$ which the ion travels, in the time t_0 required to

strike the plate, differs somewhat from this. In fact, the criterion for striking the plate is simply

$$z(t_0) = z_0 + y(t_0) \cot \theta_B .$$

The second term, which gives the effect due to gyromotion, can have either sign.

If $\Omega(t_0)t_0 \gg 1$, many gyrations occur before the ion hits the plate. In this case it is simpler to consider the orbit as defining a funnel, and to calculate the point at which the funnel intercepts the plate. Then the criterion is simply

$$z(t_0) = z_0 - \frac{[v_x^2(0) + v_y^2(0)]^{1/2} + v_x(0)}{\Omega} \cot \theta_B ,$$

and of course the ion strikes the plate before it travels the full distance along the field line.

REFERENCES

1. J. N. Brooks, J. Nucl. Mater. 111 & 112, 457-458 (1982).
2. K. L. Bell, et al., "CLM-R 215, Culham Laboratory (1982).
3. M. Thompson, Philosophical Magazine 18, 377 (1968).
4. J. A. Schmidt, et al., "USFED-INTOR Activity," Chapt. VI, USA-FED-INTOR/82-1 (1982).
5. D. E. Post, et al., Atomic Data and Nuclear Data Tables 20, 397 (1977).

Distribution for ANL/FPP/TM-171

Internal:

M. Abdou	A. Hassanein	R. Mattas
C. Baker	K.-N. Huang	B. Misra
E. Beckjord	M. Inokuti	R. Nygren
C. Boley	C. Johnson	J. Roberts
J. Brooks	J. Jung	D. Smith
F. Cafasso	M. Kaminsky	A. Stehney
Y. Cha	S. Kim	H. Stevens
R. Clemmer	Y.-K. Kim (2)	L. Turner
D. Ehst	R. Kustom	R. Wehrle
K. Evans	R. Lari	ANL Patent Dept.
P. Finn	L. LeSage	FP Program (25)
Y. Gohar	B. Loomis	ANL Contract File
L. Greenwood	S. Majumdar	ANL Libraries (2)
D. Gruen	V. Maroni	TIS Files (6)

External:

DOE-TIC, for distribution per UC-20, -20g (165)

Manager, Chicago Operations Office, DOE

Special Committee for the Fusion Program:

S. Baron, Burns & Roe, Inc., Oradell, NJ
H. K. Forsen, Exxon Nuclear Company, Inc., Bellevue, WA
M. J. Lubin, Standard Oil Company of Ohio, Warrensville Heights, O
G. H. Miley, University of Illinois, Urbana
P. J. Reardon, Princeton University
D. Steiner, Rensselaer Polytechnic Institute
K. R. Symon, University of Wisconsin-Madison
K. Thomassen, Lawrence Livermore National Laboratory
B. Dewald, Georgia Institute of Technology
D. Hefetz, Princeton Plasma Physics Laboratory
R. McGrath, Pennsylvania State University
D. Post, Princeton Plasma Physics Laboratory
Library, Centre de Etudes Nucleaires de Fontenay, France
Library, Centre de Etudes Nucleaires de Grenoble, France
Library, Centre de Etudes Nucleaires de Saclay, France
Library, Centre de Recherches en Physique des Plasma, Lausanne, Switzerland
Library, FOM-Institute voor Plasma-Fysika, Jutphass, Netherlands
Library, Comitato Nazionale per l'Energia Nucleare, Rome, Italy
Library, Joint Research Centre, Ispra, Italy
Library, Japan Atomic Energy Research Institute, Ibaraki, Japan
Library, Max Planck Institute für Plasmaphysik, Garching, Germany
Library, Culham Laboratory, UKAEA, Abingdon, England
Library, Laboratorio Gas Ionizzati, Frascati, Italy