Subroutines for some plasma surface interaction processes: physical sputtering, chemical erosion, radiation enhanced sublimation, backscattering and thermal evaporation

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Abstract
A suite of FORTRAN subroutines/functions to generate data using empirical formulas for physical sputtering of monoatomic targets for any elemental incident ion (atom), chemical erosion of graphite, Radiation Enhanced Sublimation (RES) of graphite, the number and energy backscattering coefficients for any elemental incident ion (atom) on a compound target and thermal evaporation of graphite is presented. Since chemical erosion, RES and thermal evaporation depend on the surface temperature of graphite, a subroutine implementing the 1-D heat diffusion equation to determine the temperature of any plasma-facing graphite surface is implemented. As an example to illustrate the use of these subroutines/functions, a simple model for the erosion of a plasma-facing surface, consisting of a simple collisionless sheath model, a 1-dimensional steady state heat diffusion model and 0-dimensional steady state particle balance at the target is developed and a sample listing of the program is presented.

Program summary

Title of program: Plasma Surface Interaction Codes (PSIC)
Catalog identifier: ADTR
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADTR
Program obtainable from: CPC Program Library, Queen’s University of Belfast, N. Ireland
Computers for which the program has been designed for and others on which it has been tested: Program is designed for any computer with a FORTRAN-77 compiler. It has been tested on a Linux PC with g77, Absoft f77, f90, f95, Fujitsu f95, Lahey f95
Operating systems under which the program has been tested: Linux, UNIX
Programming language used: FORTRAN-77
Memory required to execute with typical data: Negligible (executable is 178 861 bytes; add to it the memory used by the Fortran library linked to)

∗ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).
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1. Introduction

Plasma Surface Interactions (PSI) are important in any plasma device, be it plasma processing, fusion devices or any experiment studying basic plasma physics. It is necessary to quantify the various PSI processes like sputtering, backscattering, recycling from the walls, etc. in order to see the effect of these on the plasma, and on the plasma-facing surface. At times, a large amount of sputtering or a controlled amount of sputtering may be favourable (like in plasma-assisted sputter deposition) whereas in plasma-induced ion implantation, tokamaks, etc., one would like to keep the sputter erosion at a minimum. Therefore PSI data is essential to determine the target conditions and the plasma conditions to favour the task at hand. A large amount of work is dedicated to determining various PSI data by experiments and Monte Carlo codes. These data are then made available as data sets [1–3] which can be used as inputs for plasma codes or semi-empirical formulas are developed to fit the available data ([4,5] and references therein).

The data sets are available for a large number of projectile-target combinations. They are accurate and are used in existing transport codes [6–10] with a suitable interpolation to parameters of interest. However they cannot be extended to projectile-target combinations for which data are not available. The semi-empirical formulas on the other hand are not as accurate, but they have been developed by identifying the physical parameters on which the PSI processes depend and are fitted to the experimental and code-generated data, and therefore can be extrapolated to projectile-target combinations for which such data sets are not available. Using an empirical formula might also be computationally faster compared to doing a multidimensional sorting and interpolation on a large data set, especially for code packages which use PSIs as boundary conditions at each iteration. Some of these formulas are usually included in the existing transport codes [6–10].

We have implemented published semi-empirical formulas for physical sputtering [11], chemical erosion [12] and radiation enhanced sublimation (RES) [13] as FORTRAN subroutines. The number backscattering coefficient ($R_N$) and energy backscattering coefficient ($R_E$) [14,15] are calculated using a code listing published by R. Ito et al. [14] which we modified for higher ‘incident atomic weight’ to ‘target atomic weight’ ratios as described by T. Tabata and R. Ito [15]. Graphite is a widely used material in fusion devices, and chemical erosion and RES depend on the temperature of the graphite. We therefore solve the steady state 1-D heat
diffusion equation for graphite so that the surface temperature can self-consistently be estimated from the plasma parameters at the surface. We also have implemented a subroutine to calculate the thermal evaporation of graphite which becomes important at high heat loads. The chemical sputtering formulas are valid for H, D and T incident on graphite while the RES empirical formula is valid for any projectile incident on graphite. The physical sputtering formula is valid for any incident ion (atom) on any monoatomic target. The backscattering subroutines are valid for any incident ion (atom) on any compound or monoatomic target. Other PSIs like arcing, blistering and particle recycling from targets and PSI with mixed material targets are beyond the scope of this paper.

We would like to make available these FORTRAN subroutines for physical sputtering, chemical erosion, RES, backscattering, thermal evaporation and heat diffusion since it is useful to have them at a single location. We present a simple model to illustrate how these subroutines can be called and would like to make clear that the model is not valid for fully quantitative simulation of experiments. We expect the end users of these subroutines to create appropriate models when using them. However the simple model is useful to study coupled plasma surface interaction effects qualitatively which can show up also in more complex exact models [16].

The structure of the paper is as follows. In the next section we present a brief overview of the PSI mechanisms considered. In the third section we describe the subroutines. The fourth section describes a simple model for PSI which consists of a simplified sheath model with the surface interaction part being taken care of by the subroutines we provide. Section 5 describes the implementation of the simple model thereby demonstrating the installation and usage of the subroutines. Finally we present our conclusions.

2. Overview of PSI mechanisms for which subroutines are provided

In this section we briefly describe the various PSI processes for which subroutines are provided. These PSIs are classified based on the underlying physical processes they depend upon. The various parameters which they depend on are listed and this makes clear some of the input variables to the corresponding subroutine calls.

2.1. Description of the processes

When an energetic ion (atom) is incident on a surface, initially it transfers its momentum to a target atom called the primary knock-on atom (PKA). The incident atom can either lose momentum in subsequent collisions and finally come to rest in thermal equilibrium with the target (implantation) or get reflected from the target (backscattering). The PKA creates a collision cascade within the target and some of the cascading atoms can reach the surface of the target. If the atoms that reach the surface have more energy than the surface binding energy of the target material, they escape from the surface (physical sputtering). The cascading atoms also cause a lot of damage to the target and can create interstitial carbon atoms in case of a graphite target. At high temperatures (> 1200 K) these interstitial carbon atoms diffuse along the damage sites or voids in graphite, and reach the graphite surface and get desorbed thermally (radiation enhanced sublimation). A detailed introduction to physical sputtering and RES may be found in Ref. [17].

In case of a graphite target, the implanted atom which has equilibrated with the target can undergo chemical reactions [18] to form new molecules. These molecules can then diffuse to the target surface and can either get desorbed by incident atoms or be released thermally from the surface depending on the surface temperature (chemical erosion) [12]. Recently a mechanism called swift chemical sputtering wherein an incoming energetic hydrogen atom or ion breaks a covalent C–C bond on the graphite surface by pushing apart the carbon atoms due to its short range repulsive potential has been described [19]. This can result in the ejection of either a carbon atom or a hydrocarbon.
All the above erosion processes which sputter target atoms out (physical sputtering, chemical erosion and RES) are described in terms of the flux of target atoms per unit flux of incident atoms (yield). \( R_N \) is quantified by the reflected particle flux per incident particle flux and \( R_E \) is quantified by the reflected energy flux per incident energy flux.

2.2. Classification of PSIs

The PSIs discussed above can be broadly classified into (Fig. 1):

- Momentum transfer processes,
- Diffusive processes,
- Reactive–diffusive processes.

The momentum transfer processes (physical sputtering and backscattering) depend on:

1. Atomic masses of the projectile and target,
2. Energy of incidence of projectile,
3. Angle of incidence of projectile,
4. Surface roughness of the target.

The diffusive processes (RES) and the reactive diffusive process (chemical erosion) depend on:

1. The projectile mass,
2. The energy of the incident particle,
3. The target temperature,
4. Incident flux of particles.

RES also depends weakly on the angle of incidence, but chemical erosion is not dependent on the angle of incidence. RES is observed only in carbon and carbon-based materials. Carbon atoms are emitted with an isotropic angular distribution, even for grazing ion incidence and with an energy distribution equal to the surface temperature [13]. Graphite undergoes chemical erosion when hydrogen isotopes or oxygen are incident on it. Synergistic effects are seen when helium ions or electrons are incident on graphite along-with hydrogen neutrals [13]. These synergistic effects and the effect of chemical erosion due to oxygen incidence are not reflected in the

![Fig. 1. Classification of plasma surface interactions.](image-url)
empirical formulas. It must also be noted that there exists uncertainty in the flux dependence of chemical erosion due to assumption of a constant $D/XB$ values in experiments [20]. However Bayesian statistical studies [21] and molecular dynamics studies [22] suggest that a flux dependence does indeed exist for chemical erosion.

It is seen that thermal evaporation is an important erosion mechanism above 2700 K [23] for graphite. Usually the plasma-facing graphite temperatures in tokamaks and other high energy plasma confinement devices are less than 2700 K, but during thermal spikes like ELMs or during disruptions, a high heat flux is deposited in a localised region which can cause thermal evaporation to become the dominant erosion mechanism. Thermal evaporation depends on the target surface temperature.

Therefore we see that surface temperature is an important aspect of modelling plasma surface interactions like chemical erosion, RES and thermal evaporation. We include a self-consistent determination of the surface temperature as part of our PSI model (Section 4).

3. Description of the subroutines

In this section we describe the input and output variables of the subroutines and functions provided. Details of the empirical formulas used are presented in Appendix A. We mention here the changes we incorporate in order to make the subroutines well engineered (for example: We make sure that the inputs are within valid limits and we also take care that unphysical values like a negative sputtering yield at energies of incidence below the physical sputtering threshold are not returned). Note that all the variables are in double precision unless otherwise specified.

3.1. Subroutine for physical sputtering

Subroutine physput(theta, eo, z1, z2, am1, am2, es, tgdns, yldphy) implements the empirical formula for physical sputtering as described in [11] (see Appendix A.1). The inputs to the subroutine are:

- theta, the angle, in degrees, defined by the incident particle direction with the normal to the target surface.
- eo, the kinetic energy of the incident particle in eV.
- z1, the atomic number of the incident particle.
- z2, the atomic number of the target atoms.
- am1, the atomic weight in amu of the incident particle.
- am2, the atomic weight in amu of the target atoms.
- es, the surface binding energy in eV of the target.
- tgdns, the density in grams per cubic cm of the target.

The output from the subroutine is yldphy, the physical sputtering yield $Y_{phy}$. The formula implemented in physput is valid for atoms/ions hitting a monoatomic target. The angular dependence included is valid strictly only for light atoms/ions. It is extended for heavy atom/ion scattering using [24]. At the energy threshold for sputtering the formula blows up. We have however implemented the formula in such a way that the blow-up is detected and the sputtering yield goes smoothly to zero below the energy threshold. See the comments in the code for details. There exists new fit formulas for physical sputtering [3,25] which give a better description of the yield data, especially near the energy threshold and also for low mass ratios for the angular dependence. However the fit parameters are available only for a small number of all possible projectile-target combinations and not for any projectile-monoatomic target combination as the empirical formula which is currently implemented.
3.2. Functions for backscattering

Function reion(theta, energy, nz1, m1, ne, nz2, nw) and function rnilon(theta, energy, nz1, m1, ne, nz2, nw) are the functions in the listing published in [14] modified to accommodate heavy ion backscattering as described in [15] (see Appendix A.4). The inputs to the functions are:

- theta, the angle, in degrees, made by the incident particle direction with the normal to the target surface.
- energy, the kinetic energy of the incident particle in eV.
- nz1, integer variable for atomic number of incident atom.
- m1, integer variable for the mass number of incident atom.
- ne, integer variable for the number of constituent elements in the target.
- nz2, integer array of dimension ne, to hold the atomic numbers of the constituent elements of the target.
- nw, integer array of dimension ne, to hold the relative density of constituents in the target.

These formulas are not valid at low incident energies (below 10 eV) because they do not account for the binding of projectiles chemically to the surface at low energies [26].

3.3. Subroutine for chemical erosion

Subroutine chmsput(eo, z1, z2, am1, am2, tp, gamma, yldchm) is the subroutine that implements the chemical erosion formula proposed by J. Roth [12] (see Appendix A.3). The inputs to the subroutine are:

- eo, energy of the incident H isotope in eV.
- z1, the atomic number of the incident particle.
- z2, the atomic number of the target.
- am1, the atomic weight in amu of the incident particle.
- am2, the atomic weight in amu of the target.
- tp, temperature of the target plate (K).
- gamma, incident particle flux in particles/cm$^2$/s

and yldchm, the output, is the chemical erosion yield $Y_{chem}$.

In [12] there exists a correction term $C$ for the thermal erosion which can depend either on the target temperature (at low fluxes $C = 1/(1 + 3 \times 10^7 \exp(-1.4/tp))$ or on the incident particle flux (at high fluxes $C = 1/(1 + 3 \times 10^{-23} \text{gamma})$). We decide on the switchover from low incident particle flux to high incident particle flux by equating these two relations and use the high incident flux relation when gamma is greater than $10^{30} \exp(-1.4/tp)$.

3.4. Subroutine for radiation enhanced sublimation

Subroutine ressput(eo, z1, z2, am1, am2, es, tp, gamma, yldres). This subroutine implements the empirical formula for RES proposed in [13] (see Appendix A.2). The inputs to the subroutine are:

- eo, the kinetic energy of the incident particle in eV.
- z1, the atomic number of the incident particle.
- z2, the atomic number of the target.
- am1, the atomic weight in amu of the incident particle.
- am2, the atomic weight in amu of the target.
- es, the surface binding energy in eV of the target.
• tp, temperature of the target plate (K).
• gamma, incident particle flux in particles/cm²/s

and yldres, the output, is the RES yield $y^{RES}$.

### 3.5. Subroutine for thermal evaporation

Subroutine thermev(tp, am2, A, B, alpha, flxthev). The inputs to the subroutine are:

- tp, temperature of the graphite plate (in Kelvin).
- am2, atomic mass of the target (in amu).
- A & B, parameters in typical vapour pressure curve (2).
- alpha, sticking coefficient.

A = $-40.181.0$ and B = $14.8$ for graphite [27]. alpha = $0.6$–$0.9$ for metals and $0.4$ for C [23]. Subroutine thermev outputs flxthev, which is the number of atoms evaporated (atoms/m²/s).

The subroutine implements the Hertz–Knudsen equation [28] for the case of a surface in vacuum:

$$
\Gamma_{\text{thev}} = \alpha \times 10^{24} \frac{P_{\text{vap}}}{\sqrt{MT}}
$$

where $\Gamma_{\text{thev}}$ is the evaporating carbon flux from the graphite (in atoms/m²/s), $\alpha$ is the sticking coefficient (dimensionless), $P_{\text{vap}}$ is the equilibrium vapour pressure of graphite (in Pascals), M is the molecular weight (in amu) and T is the graphite temperature in Kelvin.

The vapour pressure of graphite depends on the temperature of graphite and typical vapour pressure curves for various materials are given by:

$$
\log_{10} P_{\text{vap}} = \frac{A}{T} + B.
$$

A list of values for A and B for various common plasma facing materials (obtained from [27]) is available in the file thermev.f.

### 3.6. Subroutine for heat diffusion

Subroutine heatdiff(qi, qe, TL, L, A, B, Tp).

This subroutine implements the analytical solution to the simple heat diffusion model described in Section 4.2 Eq. (13). Thermal conductivity is assumed to vary as $1/(aT + b)$ and we use the expression for the temperature at the target which is same as in [29]. The inputs to this subroutine are:

- qi, incident ion heat flux (Watts/m²).
- qe, incident electron heat flux (Watts/m²).
- TL, target temperature at the cold end.
- L, thickness of the target plate (m).
- KA, parameter $a$ in the expression for conductivity which varies as $1/(aT + b)$.
- KB, parameter $b$ in the expression for conductivity.

This subroutine outputs the temperature at the target surface (Tp). Due to the simple heat diffusion model assumed, we restrict Tp to a maximum of 3000 K which is below the sublimation energy of graphite. [30] is a good reference which plots the dependence of thermal conductivities as a function of temperature for most materials relevant to thermonuclear fusion devices.
4. Simple model for treating plasma surface interactions

Any material surface facing a plasma is connected to the plasma by means of a sheath. The sheath depends on the plasma parameters like density and temperature, ambient magnetic field and applied voltage to the plasma facing surface [31]. The sheath affects the energy and angular distributions of ions incident on the plasma facing surface. The energy deposited by the plasma on the surface determines the surface temperature which is an important parameter in quantifying the chemical erosion yield, RES and thermal evaporation contributions to graphite erosion. Therefore a model for the sheath and a heat transport model in the target are important parts of modelling PSI. However detailed models for the sheath and for heat transport are beyond the scope of this paper and we present below simple models which can be used to demonstrate how to use the subroutines described above. A zero-dimensional steady-state particle balance model is used to calculate the erosion rate of a plasma-facing surface. We also do not address the issue of possible differences in the material properties of redeposited versus bulk graphite.

4.1. Simple model for the sheath

A collisionless 1-D sheath model is used, based on the results of various studies on the plasma sheath which have been compiled by Stangeby [31]. The incident energy of ions on the surface is equal to the sum of the energy with which ions enter the presheath, the energy gained in the presheath and the energy gained in the assumed collisionless sheath. For a plasma temperature $T_i$ (for ions) and $T_e$ (for electrons) at the plasma-sheath interface, the average ion energy will be a sum of:

1. the average energy per ion leaving a Maxwellian plasma $= 2T_i$,
2. energy gained by acceleration in the presheath, given by the general non-zero $T_i$ Bohm sheath criterion [32] $= T_e + \gamma T_i$,
3. energy gained by acceleration in the sheath $= Z_i \Phi$.

Note that $T_e$ and $T_i$ are all in units of eV, $\gamma$ is 1 for isothermal flow, 5/3 for adiabatic flow with isotropic pressure and 3 for adiabatic flow [31] in the presheath. The sheath potential $\Phi$ is in V and $Z_i$ is the charge of incident ions.

For a floating surface, $\Phi$ is given by [31]

$$\Phi = \Phi_{\text{float}} = \frac{1}{2} T_e \ln \left[ \frac{2 \pi m_e}{Z_i m_i} \left( 1 + \frac{T_i}{T_e} \right) \right]$$

and for a biased surface, the plasma is shielded from the applied voltage $\Phi_{\text{app}}$ by the sheath potentials at the anode $\Phi_a$ and at the cathode $\Phi_c$, such that $\Phi_{\text{app}} = \Phi_a - \Phi_c$, with $\Phi_a$ given by

$$\Phi_a = T_e \ln \left[ \frac{2e^{\Phi_{\text{app}}/T_e}}{1 + e^{\Phi_{\text{app}}/T_e}} \right].$$

Note that when $\Phi_{\text{app}} = 0$, $\Phi_a = \Phi_c = \Phi_{\text{float}}$. Therefore the bombarding ion energy is

$$E_i = T_e + (2 + \gamma) T_i + Z_i \Phi_c.$$

The incident ion flux on the surface is the same as the ion flux entering the sheath from the presheath

$$\Gamma_s = n_s C_s,$$

where $n_s = n_e = Z_i m_i$ is the plasma density at the plasma-sheath interface, and $C_s$ is the sound speed given by $((T_e + \gamma T_i)/m_i)^{1/2}$ where $m_i$ is the mass of the ion.

The heat flux deposited by ions is given by

$$q_i = \Gamma_s E_i.$$
The heat flux deposited by electrons on the surface is given by

$$q_e = 2T_e C_s n_s e^{\Phi_{\text{app}}/T_e}. \quad (8)$$

Therefore, given the plasma parameters of density $n_s$, ion temperature $T_i$ and electron temperature $T_e$ at the plasma-sheath interface, and the applied voltage $\Phi_{\text{app}}$, useful information for PSI like average energy of incidence (5), the incident ion flux (6) and the heat flux on the surface (7), (8) can be found. Note that we do not have any information of the angular distribution of the bombarding ions, which can affect physical sputtering yields and backscattering coefficients. We assume that in the absence of collisions in the sheath, all ions are accelerated to velocities much greater than their thermal velocities (typically $\sqrt{2E_i/m_i}$) and therefore are more or less normally incident on the surface if it is assumed that there are no magnetic fields present.

4.2. Simple heat diffusion model

The 3-D heat diffusion equation is given by [33]:

$$\frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + S = \rho C_p \frac{\partial T}{\partial t}. \quad (9)$$

where $T$ is the temperature, $(x, y, z)$ are the 3 Cartesian coordinates, $k$ stands for heat conductivity, $S$ is the volumetric sources or sinks of heat per unit time, $\rho$ is the density of the surface material, $C_p$ is the specific heat of the material at constant pressure and $t$ is the time variable.

A uniform, steady state plasma is assumed to be in contact with a surface. The heat diffusion into the plasma-facing surface is assumed to be 1-dimensional. The thermal conductivity dependence on temperature can be described by $1/(aT + b)$ in most cases [29]. It is also assumed that there are no bulk sources or sinks of heat. This is a valid assumption because the range of penetration of ions and electrons in the target (at most a few hundred angstroms) is negligible compared to the target size (cm) and most of the energy loss of these incident particles occurs much before the end of their range.

With these assumptions the 3-D, time dependent heat diffusion equation reduces to

$$\frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) = 0 \quad (10)$$

the steady state 1-D heat diffusion equation (without bulk volumetric sources or sinks) [33].

The heat flux incident on the surface is used to implement a Neumann-type boundary condition at the plasma-facing end $(x = 0)$

$$-k(T) \frac{\partial T}{\partial x} = q_i + q_e \quad (11)$$

where $q_i$ and $q_e$ are given by Eqs. (7), (8). Therefore, the incident heat flux on the surface enters the equations as a boundary condition which is an effective heat flux source at the boundary surface. Note that here we neglect the cooling of the surface due to radiation and evaporation or sublimation. The additional contribution to the deposited heat by ion recombination on the target is also neglected.

The temperature at the cool end $(x = L)$ is specified to implement a Dirichlet-type boundary condition

$$T(L) = T_L. \quad (12)$$

With the assumed $1/(aT + b)$ variation of $k$, and solving Eq. (10) with the boundary conditions specified by Eq. (11), (12) results in the temperature $T_p$ at the surface (as in [29]) given by:

$$T_p = \left( T_L + \frac{b}{a} \right) e^{(q_i+q_e)L} - \frac{b}{a}. \quad (13)$$
4.3. Surface interaction model

We present a 0-D steady state particle flux balance equations for surface interactions with hydrogen as the plasma species and graphite as the target. It is similar to [23], but with backscattering of the returning carbon flux considered and is also extended to calculate net erosion. The addition of backscattering of the incident carbon ions is necessary only when one can differentiate between the backscattered carbon atoms and sputtered carbon atoms. The semi-empirical formulas for sputtering yield [11] and backscattering [14,15] implies differentiation between the carbon sputtered and the carbon backscattered.

Consider an incident flux of hydrogen ions $\Gamma_H$. This results in a sputtered flux of carbon atoms. Some of this flux of carbon atoms gets ionised and returns to the target. The returning flux of carbon also causes self sputtering of graphite. A fraction $R_N$ of the returning flux of carbon atoms also backscatters from the surface, with the remaining fraction $(1 - R_N)$ getting redeposited on the target. In addition to these processes there is also a steady flux of carbon atoms evaporated from the surface. A steady state picture of all the processes involved is shown in Fig. 2. We see from the figure that in steady state the total flux of carbon atoms going away from the target is

$$\Gamma_C^{\text{out}} = Y_H \Gamma_H + Y_C \Gamma_C^{\text{ret}} + R_N \Gamma_C^{\text{ret}} + \Gamma_C^{\text{evap}}$$

(14)

where $Y_H \Gamma_H$ is the total sputtered flux of carbon atoms due to hydrogen incidence and $Y_H$ is a sum of the physical, chemical and RES yield contributions of H incident on graphite:

$$Y_H = Y_{\text{phy}}^H + Y_{\text{chem}}^H + Y_{\text{RES}}^H$$

(15)

and $Y_C \Gamma_C^{\text{ret}}$ is the total self-sputtering flux with $Y_C$ given by

$$Y_C = Y_{\text{phy}}^C + Y_{\text{RES}}^C.$$

(16)

Fig. 2. 0-D steady state surface erosion model.
$R_C^{\text{ret}}$ is the backscattered carbon flux and $\Gamma_{\text{evap}}^C$ is the evaporated flux of carbon. $\Gamma_{\text{ret}}^C$ is the fraction $f_r$ of $\Gamma_{\text{out}}^C$ that returns to the target after ionisation in the plasma.

$$\Gamma_{\text{ret}}^C = f_r \Gamma_{\text{out}}^C,$$  \hspace{1cm} (17)

$f_r$ is an external parameter which is an input to the model and should come from impurity transport calculations.

The flux of carbon atoms lost from the surface is

$$\Gamma_{\text{loss}}^C = \Gamma_{\text{out}}^C - R_C^N \Gamma_{\text{ret}}^C = Y_H \Gamma_H + Y_C \Gamma_{\text{ret}}^C + \Gamma_{\text{evap}}^C$$  \hspace{1cm} (18)

and the flux of carbon atoms redeposited by the returning carbon flux is

$$\Gamma_{\text{redep}}^C = (1 - R_C^N) \Gamma_{\text{ret}}^C.$$  \hspace{1cm} (19)

From Eqs. (14), (17) we get

$$\Gamma_{\text{ret}}^C = \frac{f_r (Y_H \Gamma_H + \Gamma_{\text{evap}}^C)}{1 - f_r (Y_C + R_C^N)}.$$  \hspace{1cm} (20)

The gross effective sputtering yield, defined as $\Gamma_{\text{loss}}^C / \Gamma_H$, using Eqs. (18) and (20) is

$$Y_{\text{eff}}^{\text{gross}} = \frac{(Y_H + \Gamma_{\text{evap}}^C / \Gamma_H)(1 - f_r R_C^N)}{1 - f_r (Y_C + R_C^N)}.$$  \hspace{1cm} (21)

The net effective sputtering yield, defined as $(\Gamma_{\text{loss}}^C - \Gamma_{\text{redep}}^C) / \Gamma_H$, using Eqs. (18)–(20) is

$$Y_{\text{eff}}^{\text{net}} = \frac{(Y_H + \Gamma_{\text{evap}}^C / \Gamma_H)(1 - f_r)}{1 - f_r (Y_C + R_C^N)}.$$  \hspace{1cm} (22)

Given a target density $n_{\text{trg}}$ (gm/cm$^3$) the gross or net thickness eroded per second (i.e., the gross or net erosion rate of the target) is given by

$$G = \frac{Y_{\text{eff}}^{\text{gross,net}} \Gamma_H M}{n_{\text{trg}} 6.0221 \times 10^{23}} \text{ (cm/s)}$$  \hspace{1cm} (23)

where $M$ is the molecular weight of the target in amu and $\Gamma_H$ is given in particles/cm$^2$/s.

This model is readily extensible to an arbitrary charge state distribution of the incoming ions and energetic neutrals, provided one accounts for all the charge states and their respective incident energies and yields separately.

5. Implementation of the simple model

A listing of a g77 (FORTRAN) program is given below to demonstrate how the various subroutines provided are used to implement the simple model for studying plasma surface interactions. Listings of an input file smpsi.inp and a makefile listing are also provided to demonstrate the compilation and linking of the main program to the subroutines in a PC running Linux. The program source is well commented and all equations specified refers to equations in this paper.
5.1. Listing of the FORTRAN program

c Main program implementing a simple model for plasma surface interactions

c Last modified by Manoj Warrier on (30-01-2003)

    implicit none

    real*8 Te, Ti, nei, Phi, Tp, theta, z1, z2, am1, am2, es, 
    & tgdns, gamma, Ei, Cs, qi, qe, TL, L, KA, KB, A, B, 
    & alpha, fr, KBoltz, MassP, Pi, MassE
    real*8 YieldPhyH, YieldChm, YieldRESH, YieldPhyC, YieldRESC, 
    & RnC, YieldH, YieldC, YEffGross, YEffNet, EroRateGross, 
    & EroRateNet, GammaInc, GammaIncC, GammaEvap, RnH
    integer i
    real*8 rnion

    parameter (KBoltz=1.3804d-16, MassP=1.6726d-24, 
    & Pi=3.141592654, MassE=9.1094d-28)

    open (2, file='smpsi.inp', status='old')
    open (3, file='smpsi.out', status='unknown')

    c Inputs to the subroutine
    c For a table of Surface binding energies and Densities of various
    c targets look in the "incatm" file provided with PSIC or run PSIC,
    c click on target atom and click on element of interest.

    read(2,*)Ti ! Plasma Ion Temperature at the Plasma- 
    ! Sheath interface (eV).
    read(2,*)Te ! Plasma Electron Temperature at the 
    ! Plasma-Sheath interface (eV).
    read(2,*)nei ! Plasma Density at the Plasma-Sheath 
    ! interface (ions/cm^3).
    read(2,*)Phi ! Applied bias voltage (Volts).
    read(2,*)theta ! Angle the projectile makes with normal 
    ! to target (degrees).
    read(2,*)z1 ! Atomic number of incident atom.
    read(2,*)z2 ! Atomic number of target atom.
    read(2,*)am1 ! Atomic mass of incident atom (amu).
    read(2,*)am2 ! Atomic mass of target atom (amu).
    read(2,*)es ! Surface binding energy (heat of 
    ! sublimation) of target (eV).
    read(2,*)tgdns ! Density of the target (gms/cm^3).
    read(2,*)L ! Thickness (cms) of the target.
    read(2,*)TL ! Temperature at the opposite end (as opposed 
    ! to plasma facing end) of the target (Kelvins).
    read(2,*)KA ! Parameter "a" in the temperature dependent 
    ! thermal conductivity profile k(T)= 1/(aT+B).
    read(2,*)KB ! parameter "b" in the thermal conductivity 
    ! profile.
read(2,*)A ! Parameter in the vapor pressure curve
! (see Eqn.2, and subroutine thermev for data
! on A and B for many plasma facing materials)
read(2,*)B ! Parameter in the vapor pressure curve
read(2,*)alpha ! Sticking coeff (0.6-0.9 for metals and
! 0.05 for C_3 and 0.4 for C).
read(2,*)fr ! Returning fraction of outgoing atoms.
read(2,*)gamma ! (depends on the type of flow assumed in
! the pre-sheath; =1 for isothermal flow,
! = 5/2 for adiabatic flow with isotropic
! pressure, = 3 for adiabatic flow) Ref.20
! of paper for more detailed info.

! Converting L into meters for subroutine heatdiff
L = L / 100.0d0

! Finding the sheath potential drop (See Eqn.3)
if (Phi.eq.0.0d0) Phi = 0.5d0 * Te * log(2.0d0 * Pii * MassE / & MassP / am1 * (1.0d0 + Ti / Te))
print*,"Sheath potential drop Phi = ",Phi," eV"

! Bombarding ion energy, Ei (in eV) (Eqn.5)
Ei = Te + (2.0d0 + gamma) * Ti - Phi
print*,"Bombarding ion energy = ",Ei," eV"

! Sound Speed (in cms/sec)
Cs = (KBoltz / MassP * (Te + gamma * Ti))**0.5
print*,"Sound Speed = ",Cs," cms/sec"

! Incident particle flux, GammaInc (in prt/cm^2/sec)
GammaInc = nei * Cs
print*,"Incident particle flux = ",GammaInc," prt/cm^2/sec"

! Heat flux deposited by ions and electrons, qi and qe,
! (in ergs/cm^2/sec) (Eqns.7,8)
qi = GammaInc * Ei * 1.6022d-12
qe = 2.0d0 * Te * GammaInc * dexp(Phi / Te) * 1.6022d-12
qi = qi * 1.0d-3 !converting from c.g.s to m.k.s
qe = qe * 1.0d-3 !converting from c.g.s to m.k.s
print*,"Ion energy flux = ",qi," Watts/m^2"
print*,"Electron energy flux = ",qe," Watts/m^2"

! Finding the temperature of the target plate, Tp (in Kelvins)
call heatdiff(qi,qe,TL,KA,KB,Tp)
print*,"Surface temperature = ",Tp," K"

! Finding the evaporated flux, GammaEvap (in atoms/cm^2/sec)
call thermev(Tp, am2, A, B, alpha, GammaEvap)
GammaEvap = GammaEvap * 1.0d-4
print*, "Evaporated flux = ", GammaEvap, " atms/cm^2/sec"

Finding the gross and net erosion yields.

Physical sputtering yield due to H ion incident on Graphite.
call physput(theta,Ei,z1,z2,am1,am2,es,tgdns,YieldPhyH)
print*, "Phys sput yield due to H ion = ", YieldPhyH

Physical self sputtering yield.
call physput(theta,Ei,z2,z2,am2,am2,es,tgdns,YieldPhyC)
print*, "Phys sput yield due to C ion = ", YieldPhyC

RES yield due to H ion incident on Graphite.
call ressput(Ei,z1,z2,am1,am2,es,Tp,GammaInc,YieldRESH)
print*, "RES yield due to H ion = ", YieldRESH

Chemical sputtering yield of H incident on graphite
call chmsput(Ei,z1,z2,am1,am2,Tp,GammaInc,YieldChm)
print*, "Chem Sput yield due to H ion = ", YieldChm

Backscattering of C incident on C
RnC = rnion(theta,Ei,nint(z2),nint(am2),1,nint(am2),1)
print*, "Backscattering coeff of C ion = ", RnC

Backscattering of H incident on target
RnH = rnion(theta,Ei,nint(z1),nint(aml),1,nint(am2),1)

Total yield due to H incidence
YieldH = YieldPhyH + YieldRESH + YieldChm

RES yield due to self sputtering.
GammaIncC = fr * (YieldH * GammaInc + GammaEvap) ! roughly
call ressput(Ei,z2,z2,am2,am2,es,Tp,GammaIncC,YieldRESC)
print*, "RES yield due to C ion = ", YieldRESC

Total yield due to C incidence
YieldC = YieldPhyC + YieldRESC

Effective gross erosion yield, (Eqn.21)
YEffGross = (YieldH + GammaEvap/GammaInc) * (1.0d0 - fr*RnC) &
/ (1.0d0 - fr * (YieldC + RnC))

Effective net erosion yield, (Eqn.20)
YEffNet = (YieldH + GammaEvap/GammaInc) * (1.0d0 - fr) &
/ (1.0d0 - fr * (YieldC + RnC))
print*, "Effective Gross erosion yield = ", YEffGross
print*, "Effective Net erosion yield = ", YEffNet

Erosion rate of target (Eqn.23)
Gross
EroRateGross = YEffGross*GammaInc*am2/tgdns/6.0221d23
EroRateNet = YEffNet*GammaInc*am2/tgdns/6.0221d23
print*,"Effective Gross erosion rate = ",EroRateGross," cms/sec"
print*,"Effective Net erosion rate = ",EroRateNet," cms/sec"

stop
end

5.2. Listing of the input file

The input file smpsi.inp.

15.0d0 !ion temp (eV)
15.0d0 !electron temp (eV)
2.0e13 !density of ions (/m^3)
0.0d0 !applied potential (Volts)
0.0d0 !angle of incidence (degrees)
1.0d0 !at. number of incident atom
6.0d0 !at. number of target atom
1.008d0 !at. weight of incident atom (amu)
12.01d0 !at. weight of target atom (amu)
7.37d0 !Target Surface binding energy (eV)
1.8d0 !Target density (gms/cm^3)
3.0 !Target thickness (cm)
300.0d0 !Target temp at cold end (K)
1.3d-5 !Parameter a - heatdiff
6.0d-3 !Parameter b - heatdiff
-40181.0d0 !Parameter A
14.8d0 !Parameter B
0.4d0 !Sticking coeff
0.0 !Returning fraction
3.0d0 !gamma (type of flow)

5.3. Listing of the Makefile

SHELL=/bin/tcsh
FFLAGS = -g
INCLUDES = -I -I/usr/include
LIBS =

FF= g77

#Rule to create .o files from .f files
.f.o:
  $(FF) -c $(FFLAGS) $(INCLUDES) *f

smpsi : smpsi.o physput.o chmsput.o ressput.o thermev.o \ heatdif.o bshevi.o
5.4. Installation, compilation and running

Copy the compressed tar file psic.tar.gz to desired location. Installation on a Linux PC or any UNIX workstation involves the following commands typed at the prompt:

- $ gunzip psic.tar.gz to uncompress the file and extract the tar archive psic.tar.
- $ tar -xvf psic.tar which creates a directory psic and extracts the archived files.

To compile, change to directory psic and edit the Makefile and set FF to your favourite FORTRAN-77 compiler and then run make at the command prompt.

For running the example program, do make run at the command prompt.

5.5. Output and discussion

The following is output onto the standard output when the simple model is run with the given input file:

Sheath potential drop $\Phi = -37.4426754 \text{ eV}$
Bombarding ion energy = 127.442675 eV
Sound Speed = 70369.1094 cms/sec
Incident particle flux = 1.40738219E+18 prt/cm^2/sec
Ion energy flux = 287371.475 Watts/m^2
Electron energy flux = 5574.08445 Watts/m^2
Surface temperature = 392.169737 K
Evaporated flux = 3.36146818E-70 atms/cm^2/sec
Phys sput yield due to H ion = 0.00752572222
Phys sput yield due to C ion = 0.0330798043
RES yield due to H ion = 4.29768766E-10
Chem Sput yield due to H ion = 0.00214897338
Backscattering coeff of C ion = 0.199683094
Input error; Correct so that gamma $\geq$ 0.0
RES yield due to C ion = 0.
Effective Gross erosion yield = 0.00967469603
Effective Net erosion yield = 0.00967469603
Effective Gross erosion rate = 1.50859241E-07 cms/sec
Effective Net erosion rate = 1.50859241E-07 cms/sec

More useful output can be obtained by appropriately putting a do loop and varying the parameter of interest (ex.: $T_e$, $T_i$, $n_i$, $T_L$, etc.). For example, scanning over the plasma ion temperature (assuming $T_i = T_e$), we plot the surface temperature of the target as a function of plasma temperature (Fig. 3) and the gross erosion rate as a function of plasma temperature (Fig. 4) for a low density ($2.0 \times 10^{13}$/cm$^3$/s) case and for a high density ($8.0 \times 10^{13}$/cm$^3$/s) case. Note that there is a range of $T_i$ wherein the gross erosion rate has a local maximum. From Figs. 3 and 5 we see that this is the range where the surface temperature of the target is ideal for maximum chemical erosion.

The local maximum suggests that there could be a plasma parameter range wherein one can see a radiative instability [34] in the region where the gross erosion yield has a negative slope. In this region as the plasma temperature decreases, the gross erosion rate would increase thereby introducing more impurity into the plasma which can decrease the plasma temperature further. When the plasma temperature falls below the local maximum for gross erosion a stabilising mechanism exists wherein the gross erosion rate decreases at lower plasma temperatures and this decreases the impurities in the plasma which could lead to higher plasma temperatures thereby giving rise to the possibility of plasma oscillations about the local maximum [35]. Therefore, using these subroutines with a plasma transport code with impurity transport, increases the scope of effects that can be studied. Such a study can clearly bring out the importance of self-consistently including the target temperature calculation in any PSI model when either chemical erosion or RES plays a part. The location of such a maximum depends on various parameters like the plasma density, temperature, surface thickness and the temperature at the cool end of the surface.

Fig. 3. Target surface temperature as a function of $T_i$. 
6. Conclusions

A set of subroutines to provide data for PSI processes like physical sputtering of any monoatomic target, number and energy backscattering coefficients of any compound target, chemical erosion of graphite, RES of graphite, have been provided for use in models of Plasma Surface Interactions. A simple model of erosion of a floating porous
graphite plasma facing component is presented to demonstrate the calls to the subroutines. These subroutines can be the “PSI” part of various edge plasma and sheath codes. These subroutines can also be used to make quick estimates of the various PSI processes.

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Appendix A. The empirical formulas for the subroutines used in this paper

We briefly present the empirical formulas implemented as subroutines as an appendix. The papers from which the empirical formulas were obtained have been referred to and these references must be consulted for details of the empirical formulas. This appendix is placed for the convenience of the users of the subroutines. Since CPC also provides the subroutines finer details of the implementation can be checked in the subroutines themselves.

A.1. Empirical formula used for physical sputtering

The physical sputtering yield \( Y^{\text{phy}} \) calculation is based on the empirical formulas compiled in [11]. The Bohdansky formula [36] is used to determine the sputtering yield for normal incidence of a projectile on a target and the procedure specified by Yamamura [24] is used to specify the angular dependence:

\[
Y^{\text{phy}}(E_0) = QS_n(\varepsilon) \left[ 1 - \left( \frac{E_{\text{th}}}{E_0} \right)^{2/3} \left( 1 - \frac{E_{\text{th}}}{E_0} \right)^2 \cos \alpha \right] f \left[ 1 - (\cos \alpha)^{-1} \right] \cos \alpha_{\text{opt}}
\]

(24)

where \( Q \) and \( E_{\text{th}} \) are fitting parameters, \( E_0 \) is the incident particle energy (eV), \( \varepsilon = E_0/E_{\text{TF}} \) is the reduced energy.

\( E_{\text{TF}} \) is the Thomas–Fermi energy (eV):

\[
E_{\text{TF}} = 30.74 \frac{M_1 + M_2}{M_2} Z_1 Z_2 \left( \frac{Z_1^{2/3} + Z_2^{2/3}}{3} \right)^{1/2}
\]

(25)

where \( Z_1, Z_2, M_1, M_2 \) are the nuclear charge and atomic mass of the projectile and target respectively.

\( S_n(\varepsilon) \) is the nuclear stopping cross-section based on the Kr–C potential, which is approximated by:

\[
S_n(\varepsilon) = \frac{0.5 \ln(1 + 1.2288e)}{\varepsilon + 0.1728e^{1/3} + 0.008e^{-0.1304}}
\]

(26)

\( Q \) and \( E_{\text{th}} \) are given by:

\[
Q = 1.633 Z_1^{2/3} Z_2^{2/3} (Z_1^{2/3} + Z_2^{2/3})^{1/3}
\]

\[
E_{\text{th}} = 7.0 (M_2/M_1)^{0.54} + 0.15 (M_2/M_1)^{1.12}
\]

where \( E_s \) is the surface binding energy (heat of sublimation), \( \alpha \) is the angle made by the incident projectile with the normal to the target surface. Yamamura’s analytical fit formulas for \( f \) and \( \alpha_{\text{opt}} \) are:

\[
f = \sqrt{E_s} \left( 0.94 - 1.33 \times 10^{-3} \frac{M_2}{M_1} \right)
\]

(29)

\[
\alpha_{\text{opt}} = \pi/2 - \alpha \left( \frac{2 \varepsilon}{E_s/\gamma E_0} \right)^{-1/2}
\]

(30)
where, $a_l$ is the Lindhard screening length ($= 0.4685 \sqrt{Z_1^{2/3} + Z_2^{2/3}}$), $n$ is the target density given in units of atoms/Å$^3$ and $\gamma$ is the maximum energy transfer factor given by $4M_1M_2/(M_1 + M_2)^2$.

### A.2. Empirical formula used for RES

RES is observed only in graphite targets and the empirical formula is implemented only for a graphite target. The formula for the RES yield was obtained from [13] which states that the energy dependence of physical sputtering could also be applied to RES, with a modified value of $Q$ given by:

$$Q_{\text{RES}} = Q + 54M_1^{1.18}e^{-0.78/T} \left(\frac{\Gamma}{10^{16}}\right)^{-0.1}$$  \hspace{1cm} (31)

where $M_i$ is the mass of incident ion (amu), $T$ is the plate temperature (eV) and $\Gamma$ is the incident ion flux (cm$^{-2}$ s$^{-1}$). $M_1 = 1$ for H$^+$. Then the RES yield is given by Eq. (24), with the value of $Q$ replaced by Eq. (31) for $Q_{\text{RES}}$.

### A.3. Empirical formula used for chemical erosion

The chemical erosion yields formulas are described clearly by Roth in Appendix A of [12]. Chemical erosion consists of two contributions, one the thermal part $Y_{\text{therm}}$ and the other the surface part $Y_{\text{surf}}$,

$$Y_{\text{chem}} = Y_{\text{therm}}(1 + D Y_{\text{dam}}) + Y_{\text{surf}}.$$  \hspace{1cm} (32)

The thermal erosion is enhanced by the damage production due to incident ions $Y_{\text{dam}}$. $D$ is given by $250/M_1$ where $M_1$ is the mass of the incident hydrogen isotope. The thermal erosion is obtained by the formula

$$Y_{\text{therm}} = C_{\text{sp}^3} \frac{0.033e^{-E_{\text{chem}}/KT}}{2 \times 10^{-32} \Phi + [1 + \frac{2 \times 10^{29}}{\Phi}e^{-E_{\text{chem}}/KT}]e^{-E_{\text{chem}}/KT}}$$  \hspace{1cm} (33)

where $KT$ is the target surface temperature in eV and $C_{\text{sp}^3}$ is given by:

$$C_{\text{sp}^3} = \frac{1}{2 \times 10^{-32} + [1 + \frac{2 \times 10^{29}}{\Phi}e^{-E_{\text{chem}}/KT}]e^{-E_{\text{chem}}/KT}}.$$  \hspace{1cm} (34)

We equate the value of $C$

$$C = \frac{1}{1 + 3 \times 10^{-14}/KT}$$  \hspace{1cm} (35)

with its value for high ion fluxes where a possible influence of hydrogenation time is taken into account

$$C = \frac{1}{1 + 3 \times 10^{-23} \Phi}$$  \hspace{1cm} (36)

in order to make a transition from low incident ion fluxes to high incident ion fluxes smoothly.

The term $Y_{\text{dam}}$ due to damage caused by incident ions is given by:

$$Y_{\text{dam}}(E_0) = QS_0 \left[1 - \left(\frac{E_{\text{dam}}}{E_0}\right)^{2/3}\right] \left(1 - \frac{E_{\text{dam}}}{E_0}\right)^2.$$  \hspace{1cm} (37)

The surface erosion term is given by

$$Y_{\text{surf}}(E_0, T) = C_{\text{sp}^3} \frac{Y_{\text{des}}(E_0)}{[1 + e^{(E_0-65 \text{ eV})/40}]}$$  \hspace{1cm} (38)
where
\[ Y^{\text{des}}(E_0) = Q S_n \left[ 1 - \left( \frac{E_{\text{des}}}{E_0} \right)^{2/3} \right] \left( 1 - \frac{E_{\text{des}}}{E_0} \right)^{2/3}. \] (39)

The values recommended in Table 1 of [12] is used for \( Q, E_{\text{des}} \) and \( E_{\text{dam}} \). For \( E_{\text{rel}} \) the value for pure carbon (= 1.8 eV) is used. \( E_{\text{th}}, E_{\text{TF}} \) and \( S_n \) are calculated from Eqs. (28), (25), (26). \( E_{\text{therm}} \) is taken as 1.7 eV.

A.4. Empirical formulas used for backscattering coefficients

The empirical formula for values of \( M_1/M_2 \leq 0.5 \) are taken from [14] and that for values of \( M_1/M_2 \) up to 4.8 are taken from [15]. For a more detailed description of the variables and the expressions used, please check these original references. The formulas for the number backscattering coefficient \( R_N \) and the energy backscattering coefficient \( R_E \) are related as follows:

\[ R_N = \frac{R_E}{r_E} \] (40)

where \( r_E \) is given in terms of the reduced energy \( \varepsilon = E_0/E_{\text{TF}} \) (see Eq. (25)):

\[ r_E = \frac{1}{1 + (\varepsilon/0.133)^{0.285} + 0.530 + (\varepsilon/85)^{-1.46}}. \] (41)

For the \( M_1/M_2 \leq 0.5 \) case, \( R_E \) is given by:

\[ R_E = \frac{0.705/f}{1 + (\varepsilon/0.047)^{0.597} + (\varepsilon/0.619)^{1.5}} \] (42)

where

\[ f = \frac{Z_1^{2/3} M_1^{-1/2} \alpha^{2(-3)/(\varepsilon+1)} \rho_a}{\rho_t} \] (43)

where \( \alpha = 1 + 1/\mu \) with \( \mu \) defined as \( \mu = (M - 2)/(M_1) \), and

\[ \frac{\rho_a}{\rho_t} = \frac{2\varepsilon/\rho_n + [1/S_L + 1/(4S_B)]^{-1}}{S_a} \] (44)

with

\[ \rho_a = \frac{\Gamma[0, (C - 1) \ln(B \varepsilon)] - \Gamma[0, -2 \ln(B \varepsilon)]}{AB} \] (45)

where \( A = 0.56258, B = 1.1776, C = 0.62680, \) and \( \Gamma \) is the upper incomplete gamma function given by:

\[ \Gamma(v, x) = \int_x^\infty e^{-t} t^{v-1} \, dt. \] (46)

\( S_L, S_B \) and \( S_a \) are given by:

\[ S_L = D \frac{\alpha^{3/2}}{\xi} S_a, \] (47)

\[ S_B = 61.47 Z_1 \alpha \mu \xi Z_2^{2/3} \left( \frac{[\ln(\varepsilon_B/(1 - \beta^2) + 1 + G/\varepsilon_B)] - \beta^2}{I_0 \varepsilon_B} \right), \] (48)

\[ S_a = 0.0793 Z_1^{2/3} \mu \sqrt{\frac{\varepsilon}{M_1}}, \] (49)
where

\[
D = 0.2617 \left(1 + Z_2^{2/3}\right)^{3/2} Z_2^{-1} A_1.
\]  

(50)

\(A_1\) is the co-efficient for electronic stopping cross-section in the semi-empirical formula of Andersen and Ziegler [37].

\[
\varepsilon_B = \frac{2m_e^2 \beta^2}{Z_2 I_0},
\]

(51)

\[
I_0 = \begin{cases} 
12 + 7Z_2^{-1} & \text{for } Z_2 < 13, \\
9.76 + 58.5Z_2^{-1.19} & \text{for } Z_2 \geq 13,
\end{cases}
\]

(52)

\[
G = \begin{cases} 
100Z_1/Z_2 & \text{for } Z_1 < 3, \\
5 & \text{for } Z_1 \geq 3.
\end{cases}
\]

(53)

For the \(0.5 < M_1/M_2 \leq 4.8\) case, the formulas from [15] are used and Eq. (40) is used to determine \(R_E\). \(R_N\) is given by:

\[
R_N = \frac{G(\varepsilon)}{f_N}
\]

(54)

where

\[
G(\varepsilon) = \frac{1}{1 + (\varepsilon/0.104)^{0.577} + (\varepsilon/0.730)^{1.5}},
\]

(55)

\[
f_N = \frac{Z_2^{2/3} \rho_a}{M_1^{1/2} \mu (1 + \mu)^2 \psi}
\]

(56)

and

\[
\psi = \frac{1 + 24.1 \mu^{-3.995}}{(1+\mu)(1.34+1) + \mu^{(1+3)(1.34+1)+0.9(\mu^2+1)(2\mu^3)(1+13.3))}}.
\]

(57)

For a compound target consisting of atoms with concentrations \(c^a, c^b, \ldots\), etc., atomic charge \(Z^a, Z^b, \ldots\), etc., and atomic masses \(M^a, M^b, \ldots\), etc., \(Z_2\), and \(M_2\) are replaced with \(Z_c\) and \(M_c\) to evaluate the value of \(\varepsilon\), where

\[
Z_c = \frac{c^a Z^a + c^a Z^b + \ldots}{c^a + c^b + \ldots},
\]

(58)

\[
M_c = \frac{c^b M^a + c^b M^b + \ldots}{c^a + c^b + \ldots}.
\]

(59)

Values of \(2\varepsilon/\rho, S_L, S_B\) and \(S_a\) for the compound target are calculated using the Bragg rule.

References


