Codes for Plasma Surface Interaction Data : Erosion

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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, range of incident particles on the surface facing the plasma, 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 may be favorable (like in plasma assisted sputter deposition) whereas in plasma induced ion deposition, divertor/limiter plates in tokamaks, etc.. one would like to keep the sputter erosion at a minimum. Therefore by PSI studies one can optimize the target conditions and the plasma conditions to favor the task at hand. A large amount of work all over the world is dedicated to determining various PSI data by experiments and Monte Carlo codes and finally putting it in the form of a semi-empirical formula so that it can easily be used in models for PSI (ref. [1, 2] and references therein).

We have created a Graphical User Interface using Tcl/Tk [3] to a set of codes which contain semi-empirical formulae for Physical sputtering [4], chemical sputtering [5] and radiation enhanced sublimation (RES) [6]. The interface and the codes are described in this report. These codes can also be used as separate subroutine calls from FORTRAN (**f77, g77, f90**, etc ..) or C (**gcc**) programs. The chemical sputtering formulae 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 on any mono-atomic target. Finally, a highly simplified example calculation of erosion of a target facing a glow discharge plasma is shown so as to demonstrate how to use these subroutines in programs.

1 Brief overview of PSI mechanisms

The main PSI mechanisms are listed below. Their mechanisms and their dependence on various parameters are described in the following sub-sections.

1. Physical Sputtering.
2. Chemical Sputtering.
3. Radiation Enhanced Sublimation (RES).
4. Particle backscattering.
5. Arcing.
6. Blistering.

1.1 Physical Sputtering

Physical sputtering (fig. 1) is the removal of atoms from a solid due to the impact of energetic particles. The process can be described as momentum transfer in a collision cascade initiated by the incident particle in the surface layer of the solid. A surface atom is ejected if its energy is greater than the surface binding energy [4].

Sputtering yield (γ) is the parameter by which sputtering is quantified. It is a measure of how many target atoms are sputtered out per incident ion (fig. [4]).

Physical Sputtering depends on:

1. Atomic mass of the projectile and target.
2. Energy of incidence of projectile.
3. Angle of incidence of projectile.
4. Structural changes of the target.
5. Surface roughness of the target.

The physical sputtering yields of Hydrogen on Iron generated using PSIC is shown in fig. 2 as a function of incident energy and in fig. 3 as a function of incident angle.

1.2 Chemical Sputtering

Chemical Sputtering (fig. 4) occurs when an incident atom reacts with the target atoms to form molecules which diffuse to the surface. These molecules then desorb from the surface with the thermal energy of the surface. Here we discuss chemical sputtering of Graphite. Depending on the chemical mechanism of hydrocarbon formation, chemical sputtering is classified into athermal sputtering and thermal sputtering. Athermal chemical sputtering dominates at low target temperatures, whereas thermal sputtering dominates at higher target temperatures and depends on the incident flux of particles [5].

Other parameters affecting chemical sputtering are:

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

Chemical sputtering, however, is not dependent on the angle of incidence. Graphite undergoes chemical sputtering when Hydrogen, Deuterium and Oxygen ions are incident on it. Synergistic effects are seen when Helium ion or electrons are incident on graphite along-with Hydrogen neutrals. These are not reflected in the empirical formulae. The chemical sputtering yield of Hydrogen on Graphite using PSIC is shown in fig. 5 as a function of incident energy and in fig. 6 as a function of target temperature.

1.3 Radiation Enhanced Sublimation

RES (fig. 7) occurs when interstitial atoms formed by the incident particles diffuse to the surface and sublimate. This 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 [6].

RES depends on :

1. The incident species.

2. The energy of the incident particle.

3. The target temperature.

4. The angle of incidence of the incident particle. This dependence is weak.

5. The incident flux of particles.

1.4 Backscattering

Backscattering (fig. 7) occurs when incident particles bounce back from the target after single/multiple collisions in the target. The number of particles that bounce back per incident particle is called the particle backscattering coefficient and the ratio of the average energy with which they bounce back to the incident energy is called the energy backscattering coefficient [7, 8].

Backscattering depends upon :

1. Atomic mass of the projectile and target.

2. Energy of incidence of projectile.

3. Angle of incidence of projectile.

4. Structural changes of the target.

5. Surface roughness of the target.

1.5 Arcing

Arcing depends upon [9] :

1. Wall Conditioning
2. The space charge potential between the plasma and the wall.

Present day tokamaks have eliminated arcing by good wall conditioning. Treatment of arcing using empirical formulae is out of the scope of this report.

1.6 Blistering

In reference [10] a survey of the processes of Plasma Surface Interaction was done. In the case of Blistering, only metals like Stainless Steel, Titanium, Copper, Aluminium, Molybdenum and Tungsten were considered. Blistering occurs due to the trapping of hot gases in the interstitial spaces of the target. Treatment of blistering using empirical formulae is out of the scope of this report.

2 Using PSIC - Plasma Surface Interaction Codes package

PSIC (fig. 10) is a user interface to generate data for physical sputtering for any incident projectile on any mono-atomic target, chemical sputtering of hydrogen/deuterium/tritium incident on graphite and RES of graphite. The scripting part of PSIC is handled by Tcl and the Graphical User Interface is handled by Tk. PSIC runs on Linux, and other UNIX operating systems which have Tcl/Tk installed. The PSI part is handled by FORTRAN subroutines. The plotting is done using gnuplot [11]. This section describes how to install and use PSIC.

Notation: Boldface is used to denote files, directories, softwares and machine names, whereas typesetting font is used for things to be typed in at the prompt and for parts of the code.

2.1 Installing PSIC

PSIC can be obtained by anonymous ftp from the pub directory at **manoj.plasma.ernet.in**. The file name is **PSIC.tar.gz**. It can be installed in the user's home directory or wherever the user has permission to do so. Do `tar -zxvf PSIC.tar.gz`. If you do not have the **GNU tar** the `-z` option above will give an error and in such a case do `gunzip PSIC.tar.gz`. This will create a file **PSIC.tar**. Then type in `tar -xvf PSIC.tar`. This will create a directory called **PSIC** which contains all the relevant files. Change directory to **PSIC**, and follow the instructions in the file **INSTALL**. It will be a good idea to read the documents in **/whereveryouinstall/PSIC/doc/**.

For a quick-start, edit the makefile to use whichever type of **FORTRAN** that is supported in your machine and type in `make all` in the **/whereveryouinstall/PSIC/** directory. Then edit the first line of the file PSIC to set the path for **wish**, the windowing shell of **Tk**. Use the `whereis wish` command if you do not know the path, or talk to your system administrator.

For example my Linux machine has the **g77** implementation of **FORTRAN** and **wish** is in the directory **/usr/bin**. Therefore the second line in the file **Makefile** will be `FF = g77`. The first line in PSIC will be #`!/usr/bin/wish -f`.

The SUN workstations at IPR have both **f90** and **f77**, and **wish** is in the directory **/usr/local/bin/wish**. To port PSIC to the SUN workstations at IPR one would first carry out the ftp process described in paragraph one of this section and type in `gtar -zxvf PSIC.tar.gz` command in the **/whereveryouinstall/** directory. **gtar**, which is the GNU version of **tar** is in **/usr/local/bin/** on the IPR SUN workstations. Then change directory to **/whereveryouinstall/PSIC/** directory and edit the second line of the Makefile to contain `FF = f77` and type in `make all`. Then edit the first line of the file **PSIC** to contain #`!/usr/local/bin/wish -f`. Now type `PSIC` at the prompt to start the user interface, and read the section below if you need help in using PSIC.

2.2 Using PSIC

The main window of PSIC (fig. 10), titled **PSIC** contains buttons which have to be clicked to choose

- the incident ion.
- the target.
- the PSI of interest (physical sputtering, chemical sputtering, RES).
- exiting the GUI.

Take your mouse pointer to the required choice and single click the left mouse button. *All clicks of the mouse button mentioned from here will mean the left mouse button unless otherwise specified.*

Clicking on the **Choose Incident ion** button opens up a window titled **incion** (fig. 11).

The abbreviation of all the elements in the periodic table is arranged in a column (called list-box in **Tk**) on the left side of the window **incion**. The right side of **incion** has the **Atomic number** and **Atomic weight** fields and an **OK** button. The incident ion is chosen by a double click of the left mouse button after taking the mouse pointer to the element of choice. There is a scrollbar in the listbox which can be used to view all the elements. The atomic number and the atomic weight fields (read boxes) get filled automatically when you choose the incident ion by double clicking on it. Finally a single click on the **OK** button shuts the **incion** window.

A single click on the **Choose target** button in the main window of PSIC opens a window titled **target** (fig. 12). This window too contains a listbox of all the elements of the periodic table with a scrollbar on the right to navigate through the listbox. On the right side of the listbox you have the **Atomic Number**, **Atomic Weight**, **Sublimation Energy** and **Target Density** fields. Double-clicking on any element in the listbox chooses the target and also fills up these fields. Make sure to choose a solid, else you will get unrealistic results. The target window too has a **OK** button having the same function as the **incion** window.

After choosing the incident ion and target click on the PSI of interest (physical sputtering, chemical sputtering or RES). Clicking on **Physical Sputtering** opens a window titled **ps**(fig. 13). Fields for inputing the **incident energy**, **number of data points for which data is needed**, **angle of incidence of incident ion** and finally the **range** of the independent variable for which sputtering yield needs to be found are provided. Provision to choose either **incident energy** or **incident angle** as the independent variable is provided by **radio buttons** which can be turned on by a single click. Clicking on the **accept** button causes the input file for physical sputtering to be created, the physput program to be run and the plot file **PSIC.gnu** to get setup. Clicking on the **view** button creates a plot on the screen (using **gnuplot**), and also makes a postscript file of the plot **PSIC.ps**. Clicking on the **print** button pops up a window in which you specify the postscript printer your machine is configured to print to. As soon as you specify and press enter the printing is carried out. See the file **TODO** in the **doc** directory to see how the viewing and printing aspects are going to be changed for more flexibility.

Choosing **Chemical Sputtering** in the main window of **PSIC** opens a window titled **cs** (fig. 14). **cs** is similar to **ps** except that angle of incidence can no longer be chosen as independent variable (Chemical sputtering does not show any dependence on the angle of incidence). Two new independent variables are provided as radio buttons, viz... **incident flux of particles** ($prt/m^2/s$) and **Target Temperature** (K). If any element other than Carbon is chosen as the target atom or if any atom other than H,D,T is chosen as the incident ion, a window pops up with a warning that the chemical sputtering formula is valid only for H,D,T incident on Carbon. The functioning of the **accept**, **view** and **print** buttons are similar to that in the **ps** window.

Choosing **Radiation Enhanced Sublimation** in the main window **PSIC** opens a window titled **rs** (fig. 15). The look and usage of **rs** is exactly the same as **cs**.

3 Model for sputtering and redeposition

A simplified model for a glow discharge system is presented (fig. 16). We choose the plasma species to be hydrogen and the target to be graphite (graphite shows all the three sputter mechanisms and is therefore a useful target for this illustration). It is assumed that the sheath is collisionless and the carbon that gets sputtered does not come back to the target after getting ionized. Another advantage of this assumption is that *the incident energy of ions on the target* is equal to the sum of *the energy with which they enter the sheath* and *the energy which they gain in the collisionless sheath* (=V eV for a H ion). For a plasma temperature T_i (for ions) and T_e (for electrons) in front of the target, the average bombarding energy will be a sum of:

1. The average energy of the ion just before the sheath (energy corresponding to the thermal energy) ($= \frac{3}{2}T_i$)
2. The acceleration in the pre-sheath (Bohm sheath criterion) ($= \frac{(T_e+T_i)}{2}$)
3. The acceleration in the sheath (an ion with charge Z gets accelerated to an energy ($= ZV$) in a collisionless sheath).

The bombarding ion energy works out to be $\frac{5T_e}{2} + V$ assuming singly charged ions and $T_e = T_i$.

If Γ_H is the incident flux of hydrogen atoms incident on the target and γ_C is the sputtering yield of the target at the incident energy for a specified target temperature, the flux of carbon sputtered from the graphite surface is

$$\Gamma_C = \gamma_C \Gamma_H \tag{1}$$

Carbon density is $n_C = 9.1364 \times 10^{28}$ $(atoms/m^3)$. Then the thickness eroded per second (i.e. erosion rate of the target) is given by

$$G_{ero} = \frac{\Gamma_C}{n_C} \ (meters/sec) \tag{2}$$

4 Using the subroutines in PSIC to implement the simple model

A listing of a g77 (FORTRAN) program is provided below to demonstrate how the various subroutines in PSIC are called. A makefile is also provided to demonstrate the compilation and linking of the main program to the subroutines. The example program **simple.f**, with an input file **simple.inp** and a makefile **Makefile** are provided with PSIC in the directory " /whereveryouinstall/PSIC/example".

The listing contains three calls to subroutines in the PSIC package. They are :

- `call chmsput(eo,z1,z2,am1,am2,es,Tp,gamma,yldchm,yldchath,yldchth)`
- `call ressput(eo,z1,z2,am1,am2,es,Tp,gamma,yldres)`
- `call physput(eo,z1,z2,am1,am2,es,angl,tgdns,yldphy)`

In the subroutine **chmsput**, only `yldchm, yldchath` and `yldchth` are not input variables. For a description of the rest of the variables which are input into chmsput see the program listing provided below. The listing is commented extensively. Similarly in the subroutines **ressput** and **physput**, `yldres` and `yldphy` are the only variables returned, the rest being input variables. See the program listing for a description of the input variables.

Listing of program simple.f

```
c--------------------------- simple.f ----------------------------------
c  Main program for a simple erosion model for glow discharge sputtering
c  system.
c  Last modified by Manoj Warrier on ( 31-03-2000 )

       implicit real*8(a-h,o-z)

       real*8 eo, Tplasma, angl, z1, z2, am1, am2, es, tgdns, gamma,
```

```fortran
     @  Tp, yldchm, yldphy, yldchath, yldchth, yldres
      integer numpts
      open ( 2, file='simple.inp', status='old' )

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,*)Tplasma               ! Plasma Temperature at the begining
                                     ! of the sheath (eV).
      read(2,*)V                     ! Applied Voltage (V).
      read(2,*)Tp                    ! Temperature of the target (K).
      read(2,*)gamma                 ! Incident flux of ions (Prt/m^2/s)
      read(2,*)angl                  ! incident angle of the projectile
      read(2,*)z1                    ! nuclear charge of incident atom.
      read(2,*)z2                    ! nuclear charge 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).

c  Initialising the incident energy of the ions on the target
c (=5/2*Tplasma+V)
      eo = 5.0d0/2.0d0*Tplasma+V

c  Converting target density from gms/cm^3 to prt/m^3
c  1 gram at wt of target has 6.023e23 prt.
c  => 6.023e26/am2 particles per Kg.
c  tgdns = tgdns*1.0e3 kg/m^3.
c  therefore number of prt/m^3 of target = tgdns(kg/m^3)*(6.023e26/am2)(prt/kg)
      tgdns_ppmc = tgdns*1.0d3*6.023d26/am2
```

```
c  Check for incident ion being either Hydrogen, Deuterium or Tritium,
c  and target being Carbon (because if yes we have to call chmsput
c  and RES too).
      yldchm = 0.0
      yldchath = 0.0
      yldchth = 0.0
      yldphy = 0.0
      yldres = 0.0
      if(z1.lt.2.0.and.am1.lt.4) then
          if(am2.eq.12) then
              call chmsput(eo,z1,z2,am1,am2,es,Tp,gamma,yldchm,yldchath,
     +                     yldchth)
              call ressput(eo,z1,z2,am1,am2,es,Tp,gamma,yldres)
          endif
      endif
      call physput(eo,z1,z2,am1,am2,es,angl,tgdns,yldphy)

c  Ytot is the total sputtering yield for incident ion bombarding the target
c   Note that if it is any other specie other than H/D/T incident on C,
c   Ytot=yldphy (with yldchm = yldres = 0)
      gamma_inc = gamma                   ! incident flux of ions.
      Ytot = yldphy+yldchm+yldres         ! total sputtering yield.
      Gamma_target = Ytot * gamma         ! eroded flux from target.
      Gamma_C = Gamma_target
      Erosion_rate = Gamma_C/tgdns_ppmc   !Erosion rate of target (m/s).
      write(*,*)"Erosion rate of target is = ",Erosion_rate," (m/s)"

      stop
      end
c----------------------- End of simple.f -------------------------------------
```

Given below is a sample input file for **simple.f**. It is for a Hydrogen plasma having a temperature of 3 eV at the sheath begining with a Graphite cathode which is biased at a voltage of -500 V and is at 500 K, drawing a ion flux of 1.0×10^{20}. The sublimation energy of graphite is 7.37 eV and the density is 1.80 ($gms/cm3$).

Listing of input file simple.inp

```
3
500
500
1.0d20
0.0
1.0
6.0
1.008
12.01
7.37
2.26
```

Given below is a listing of a makefile. Just go to the directory **/whereveryouin-stall/PSIC/example** and type `make` to create the executable (after changing `FF` in line 2 of the makefile to whatever **FORTRAN** you use).

Listing of Makefile

```
SHELL=/bin/bash
FF    = g77

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

simple : simple.o physput.o chmsput.o ressput.o
$(FF) simple.o physput.o chmsput.o ressput.o -o simple
```

```
simple.o: simple.f physput.f chmsput.f ressput.f

physput.o: physput.f

chmsput.o: chmsput.f

ressput.o: ressput.f

clean :
/bin/rm *.o simple
```

5 Conclusions

A set of subroutines to provide data for erosion processes like physical sputtering of any monoatomic target, chemical sputtering of graphite and RES of graphite have been provided for use in models of Plasma Surface Interaction. A Graphical User Interface also has been provided for viewing the sputtering yield with freedom to choose the incident ion, the target ion, the type of erosion process of interest and the independent variable. These subroutines have been used to find out the gross erosion rates of SST-1 and also the divertor plate temperature at which the erosion is minimum [12]. The simple model of erosion of a glow discharge cathode provided in this report is valid for a collisionless sheath. These subroutines can be the "PSI" part of a sputter deposition code, target erosion code, impurity source code, etc..

Future enhancements visualised for PSIC are :

- Include Backscattering.
- Modify the Physical sputtering yields to treat compound targets like the backscattering subroutines do. It is worth checking if such a treatment is valid because both backscattering and sputtering are two sides of the same coin!!
- Include latest formulae for chemical sputtering as proposed by J. Roth [13].

- Allow for creating parametric plots.
- Write the subroutines for PSI in C++. Tcl/Tk libraries can directly be included in C programs and the GUI will be part of the whole rather than a driver to a set of routines.
- Allow for a single data point of interest to be displayed if that is the need.
- Allow for saving the plot in whatever format one wishes and also create plots for whatever type of printer one uses other than just postscript printing.

Acknowledgements
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References

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[3] **Tcl/Tk** *Copyrighted by the Regents of the University of California, Sun Microsystems, Inc., Scriptics Corporation, and other parties.*

[4] C. Garcia-Rosales, W.Eckstien, J.Roth, *J. Nucl. Mater.*, **218** (1994) 8-17.

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[11] **gnuplot** *Copyright(C) 1986-1993 Colin Kelley, Thomas Williams.*

[12] M. Warrier, S. Jaishankar, S. P. Deshpande, et. al., *J. Nucl. Mater.*, **266-269** (1999) 726-731.

[13] J. Roth, J. Nucl. Mater. 266-269 (1999) 51-57.

Figure 1: The Physical Sputtering Process

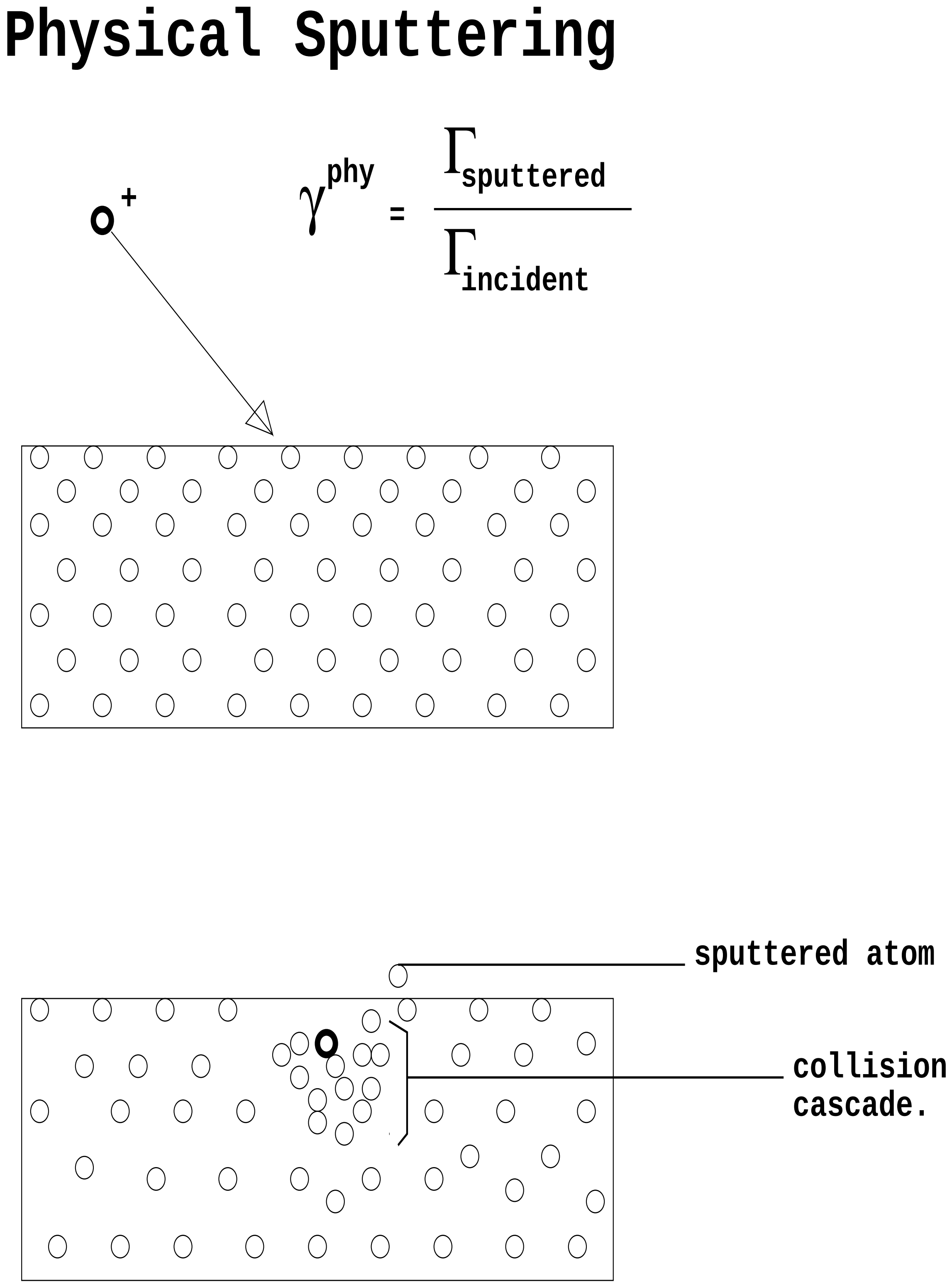

Figure 2: Physical sputtering yield of Hydrogen incident on Iron as a function of incident energy at normal incidence

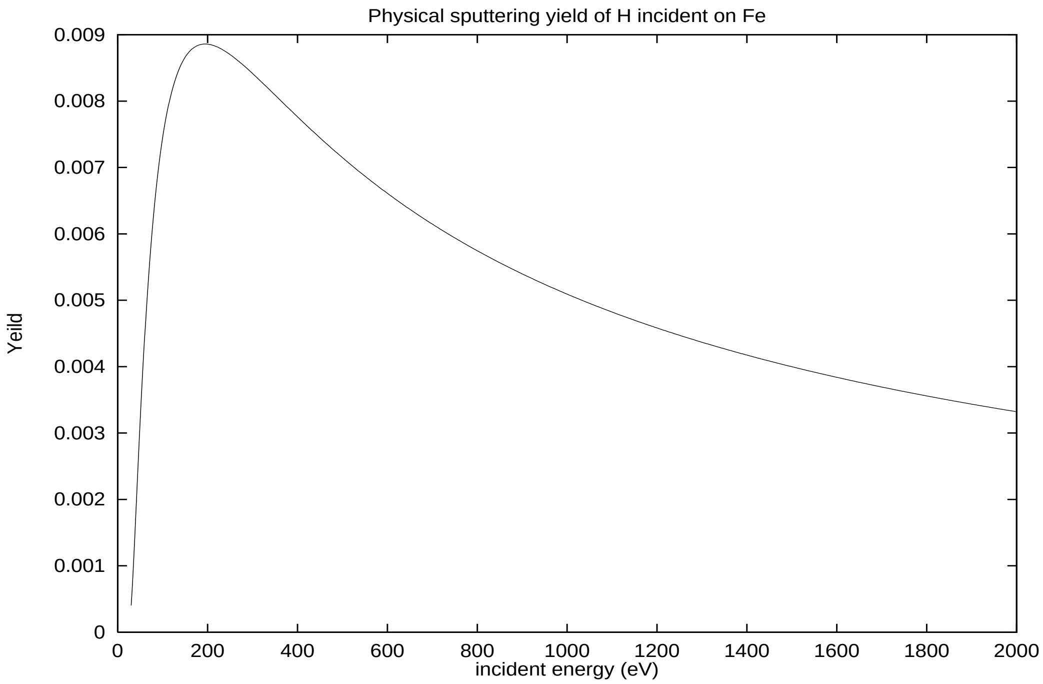

Figure 3: Physical sputtering yield of Hydrogen incident on Iron as a function of incident angle at an incident energy of 200 eV

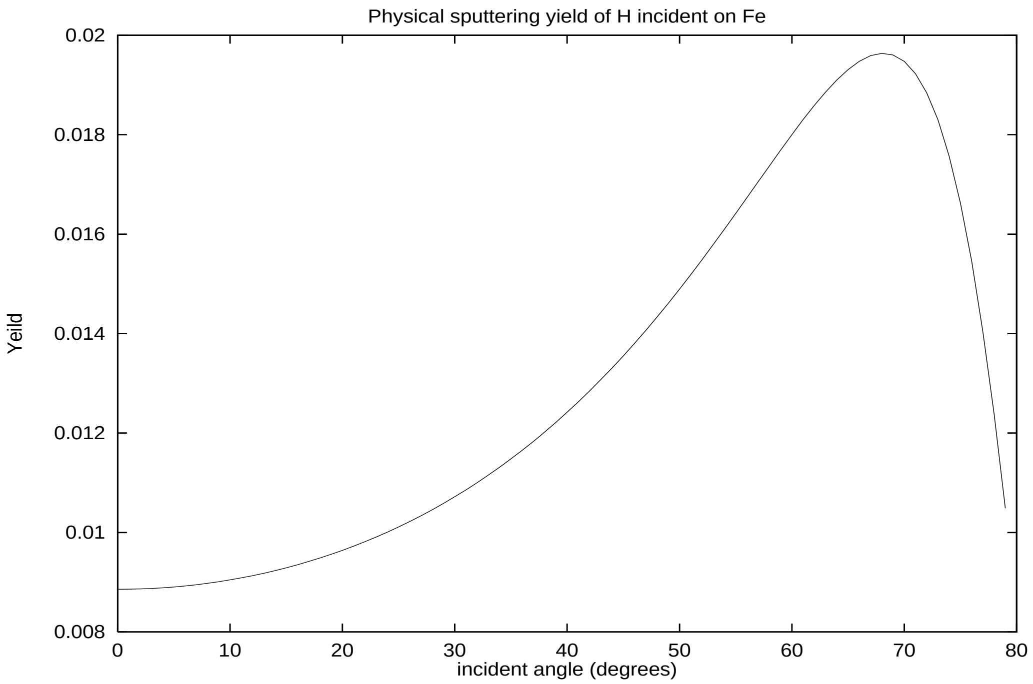

Figure 4: The chemical sputtering process

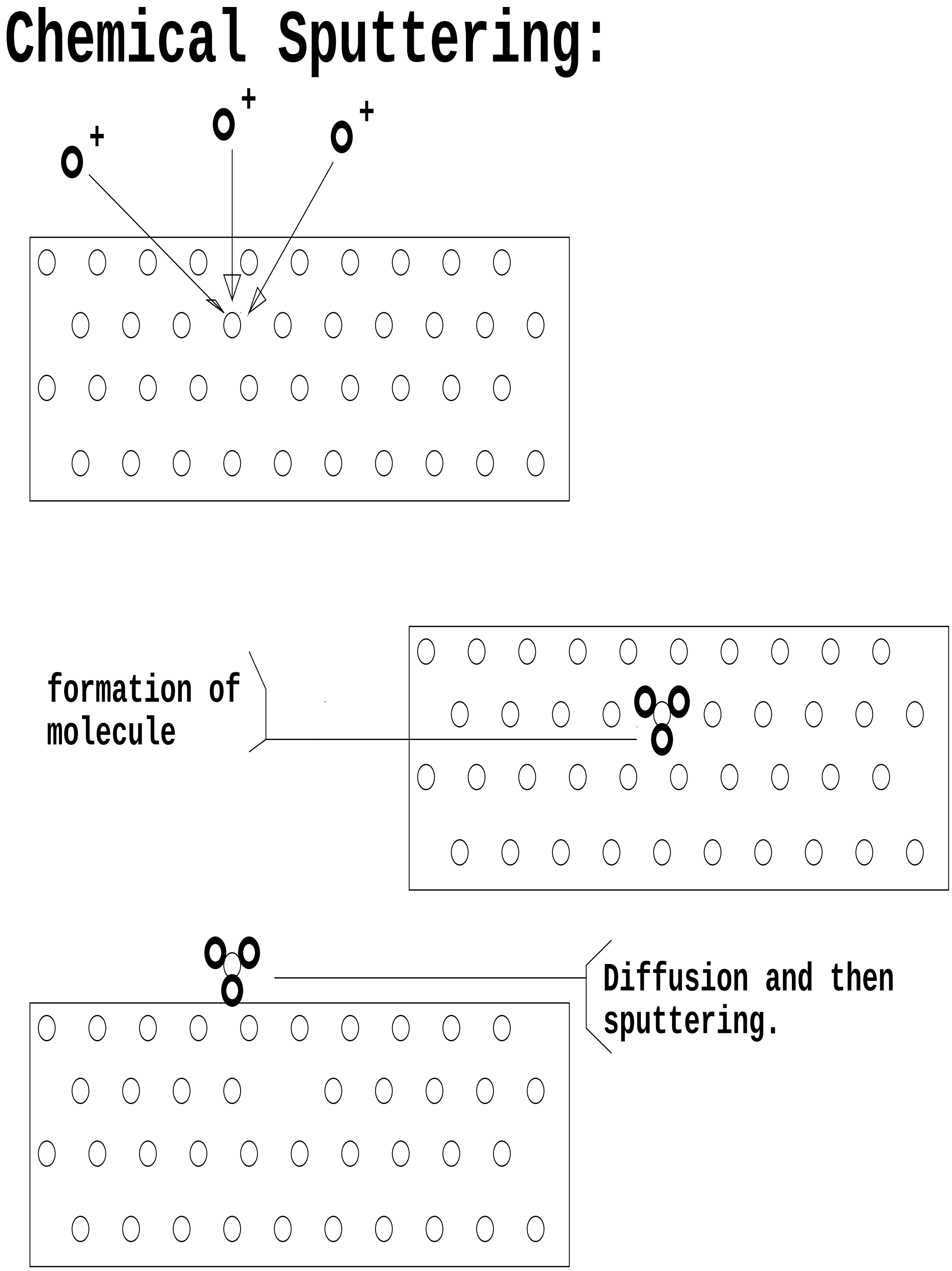

Figure 5: Chemical sputtering yields for Hydrogen incident on Graphite as a function of incident energy at a target temperature of 800 K

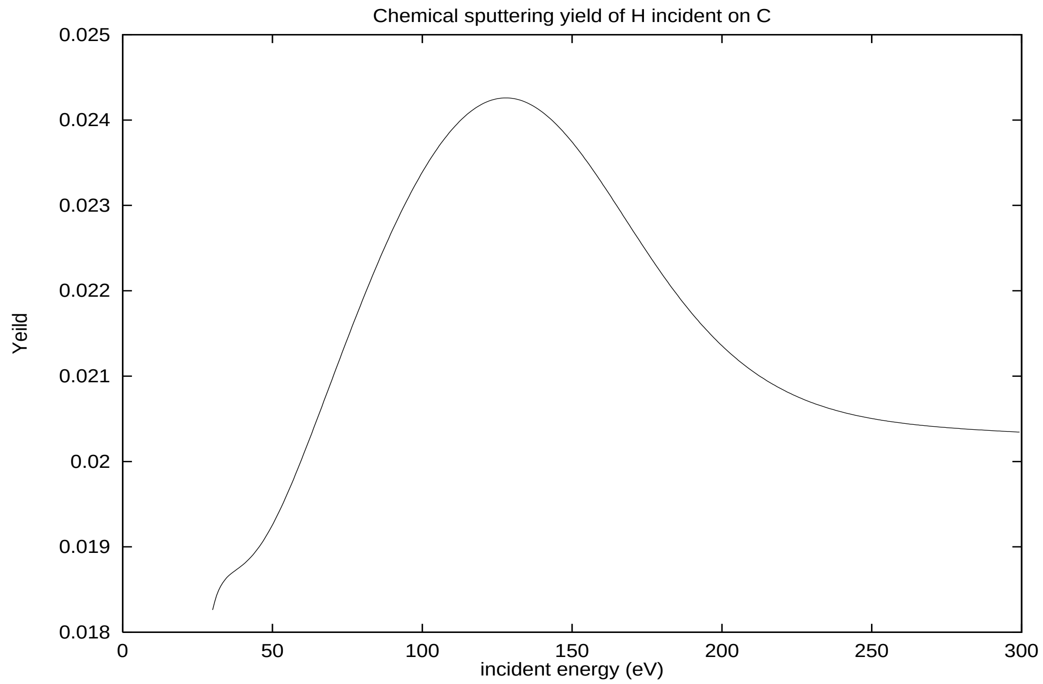

Figure 6: Chemical sputtering yields for Hydrogen incident on Graphite as a function of target temperature at an incident energy of 80 eV

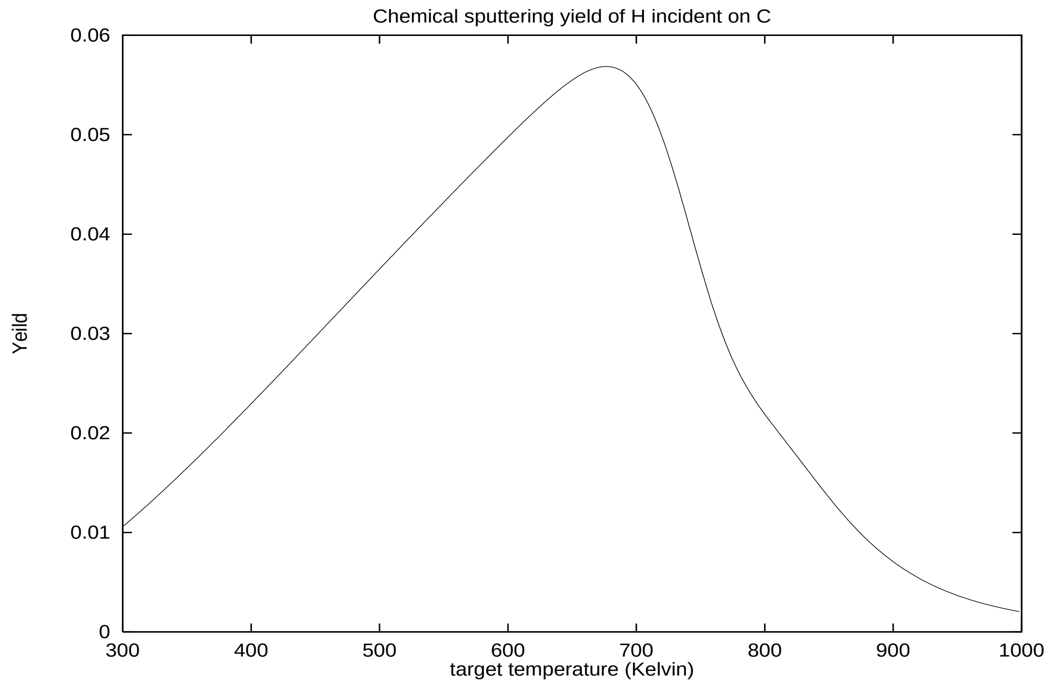

Figure 7: The radiation enhanced sublimation process

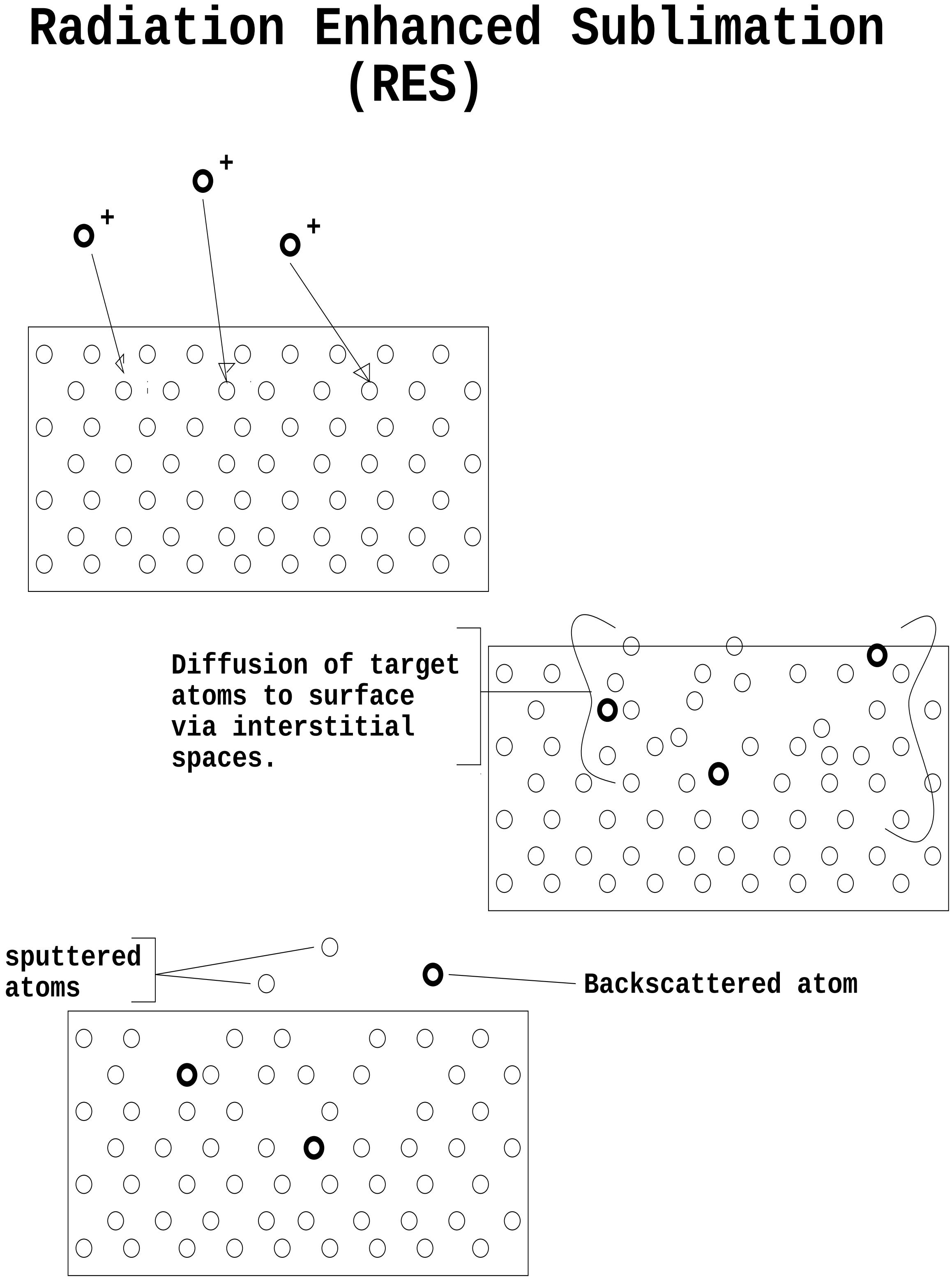

Figure 8: RES yields for Hydrogen incident on Graphite as a function of incident energy at a target temperature of 1800 K

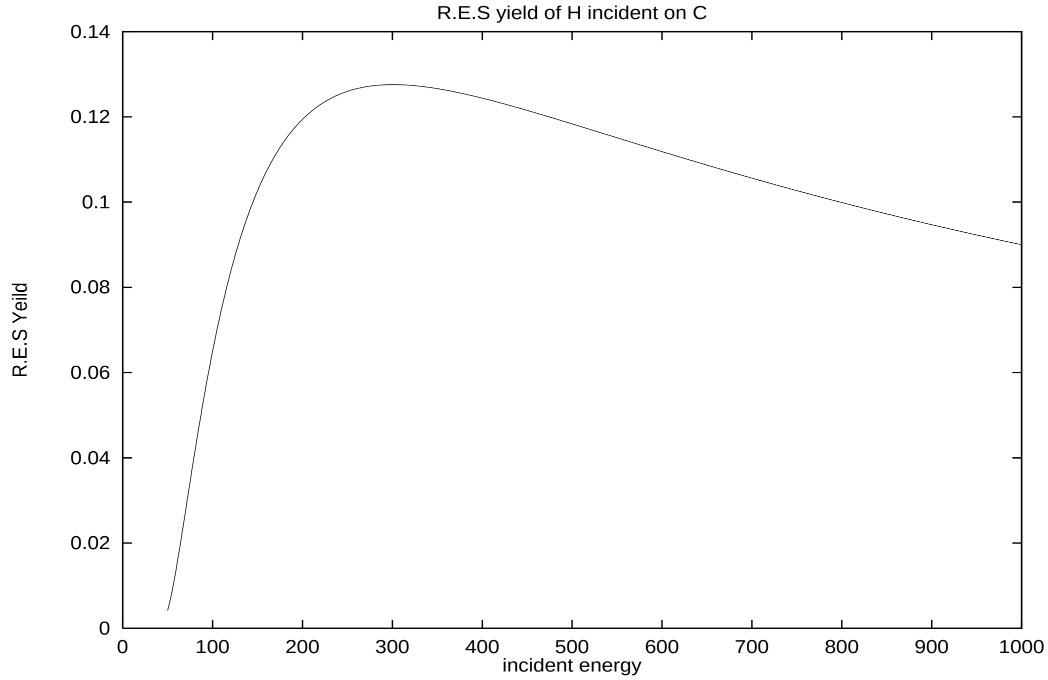

Figure 9: RES yields for Hydrogen incident on Graphite as a function of target temperature at an incident energy of 100 eV

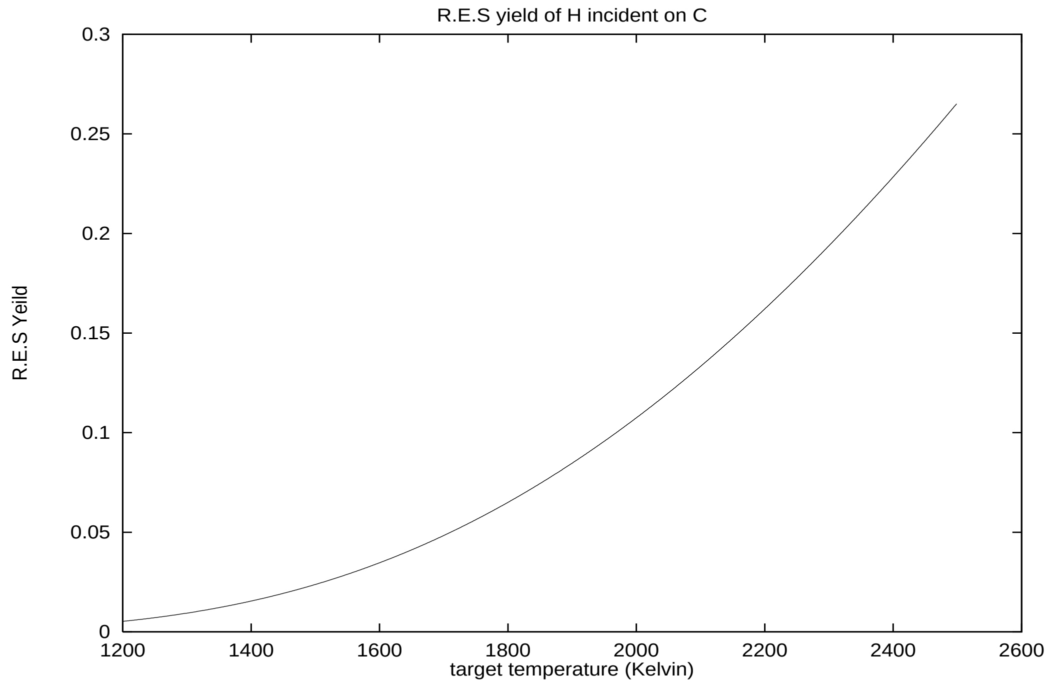

Figure 10: Main Window of PSIC

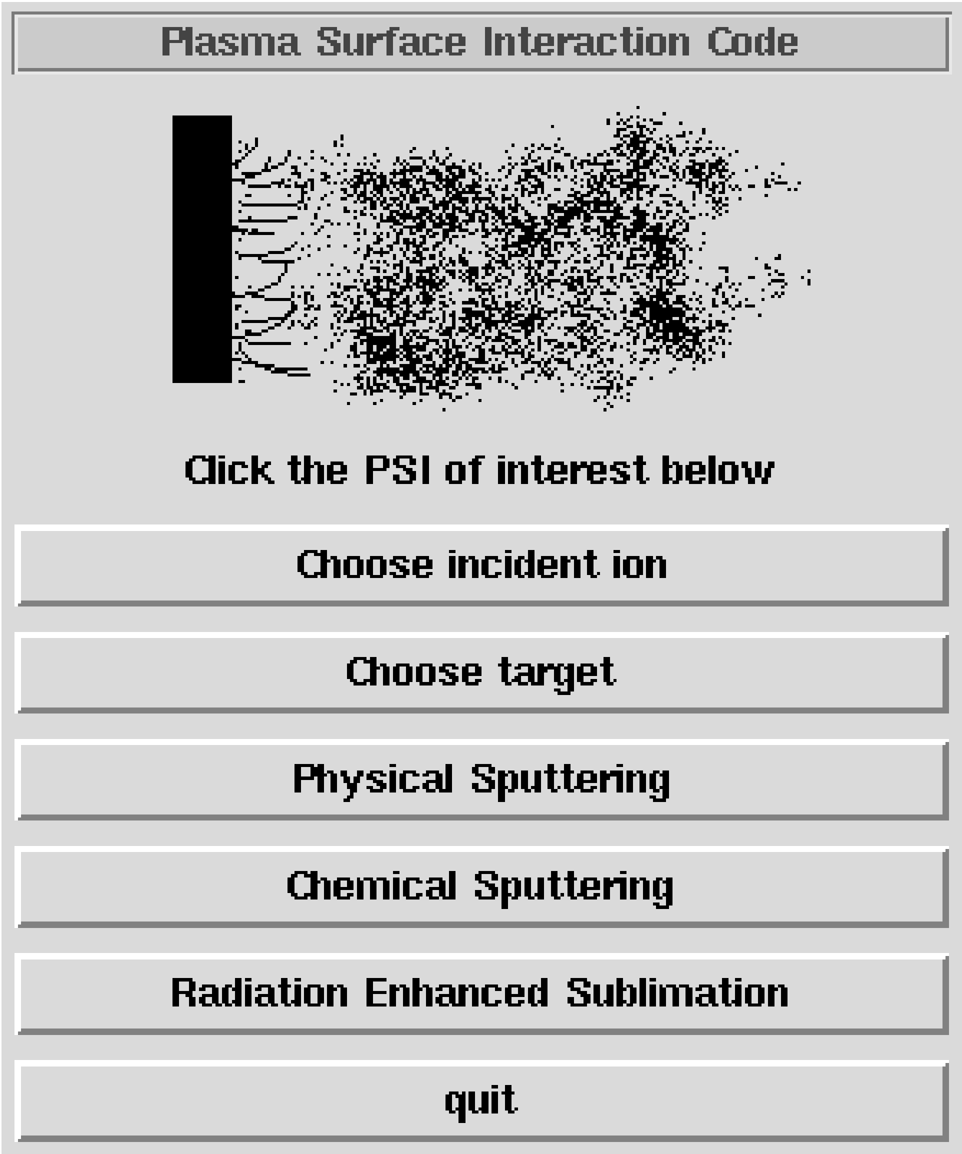

Figure 11: Window to choose the incident ion in PSIC

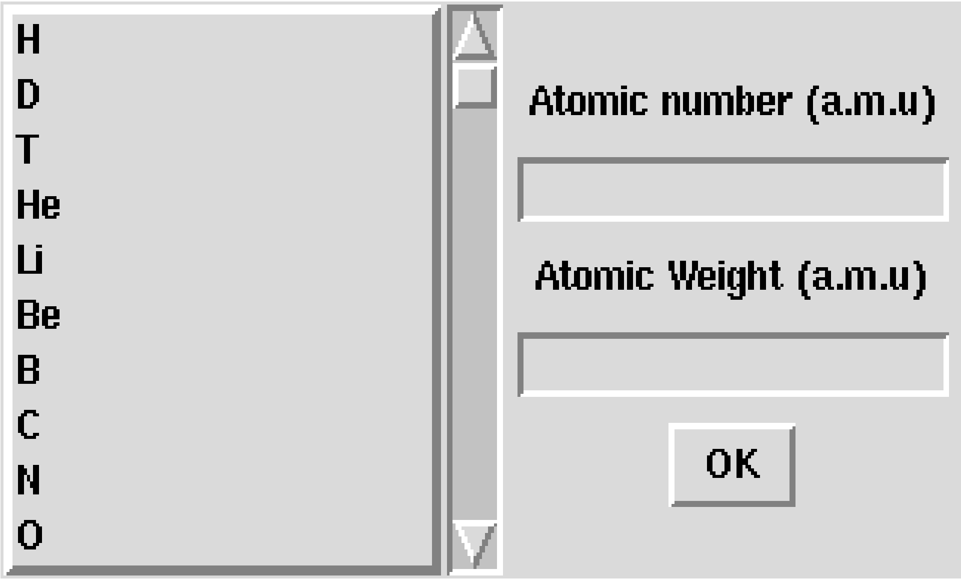

Figure 12: Window to choose the target in PSIC

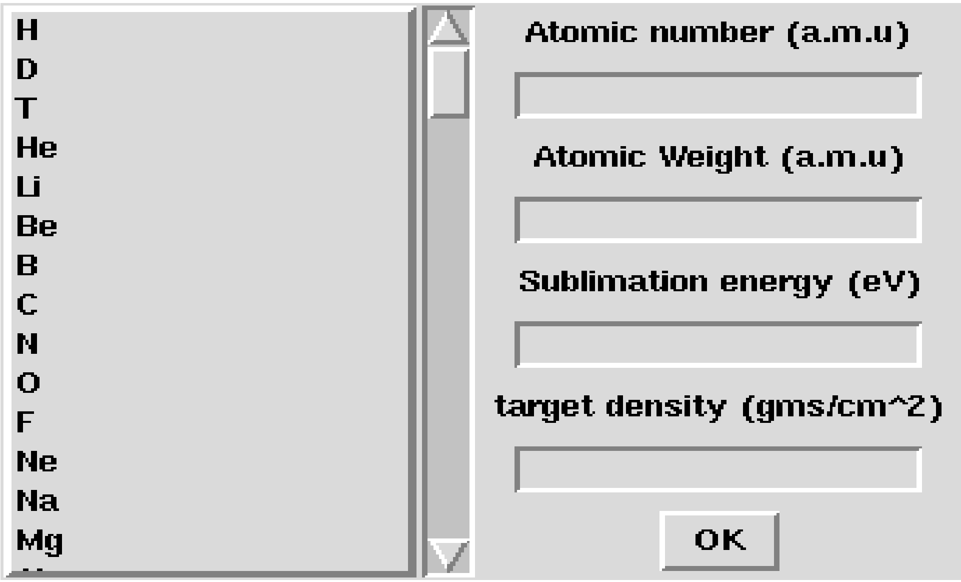

Figure 13: Window for Physical Sputtering

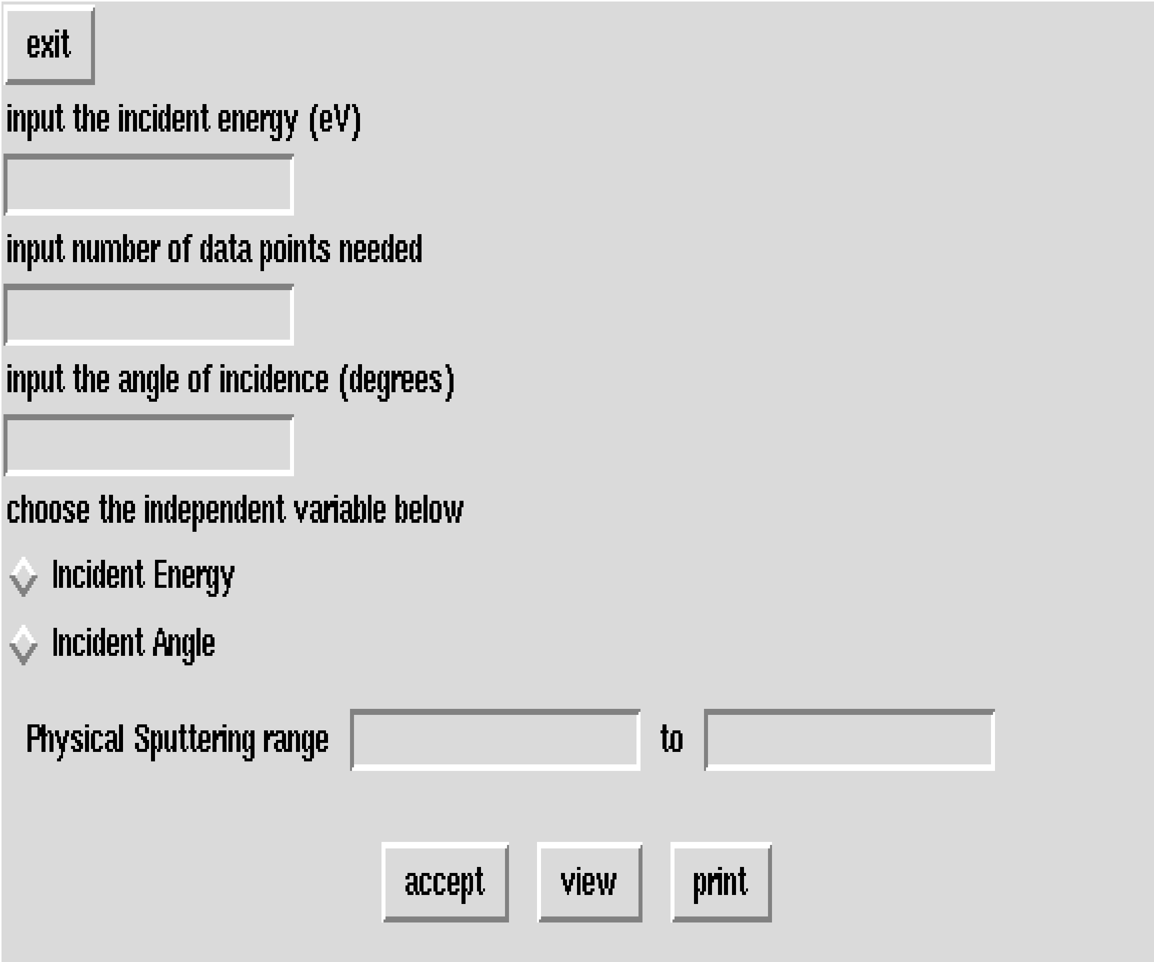

Figure 14: Window for Chemical Sputtering

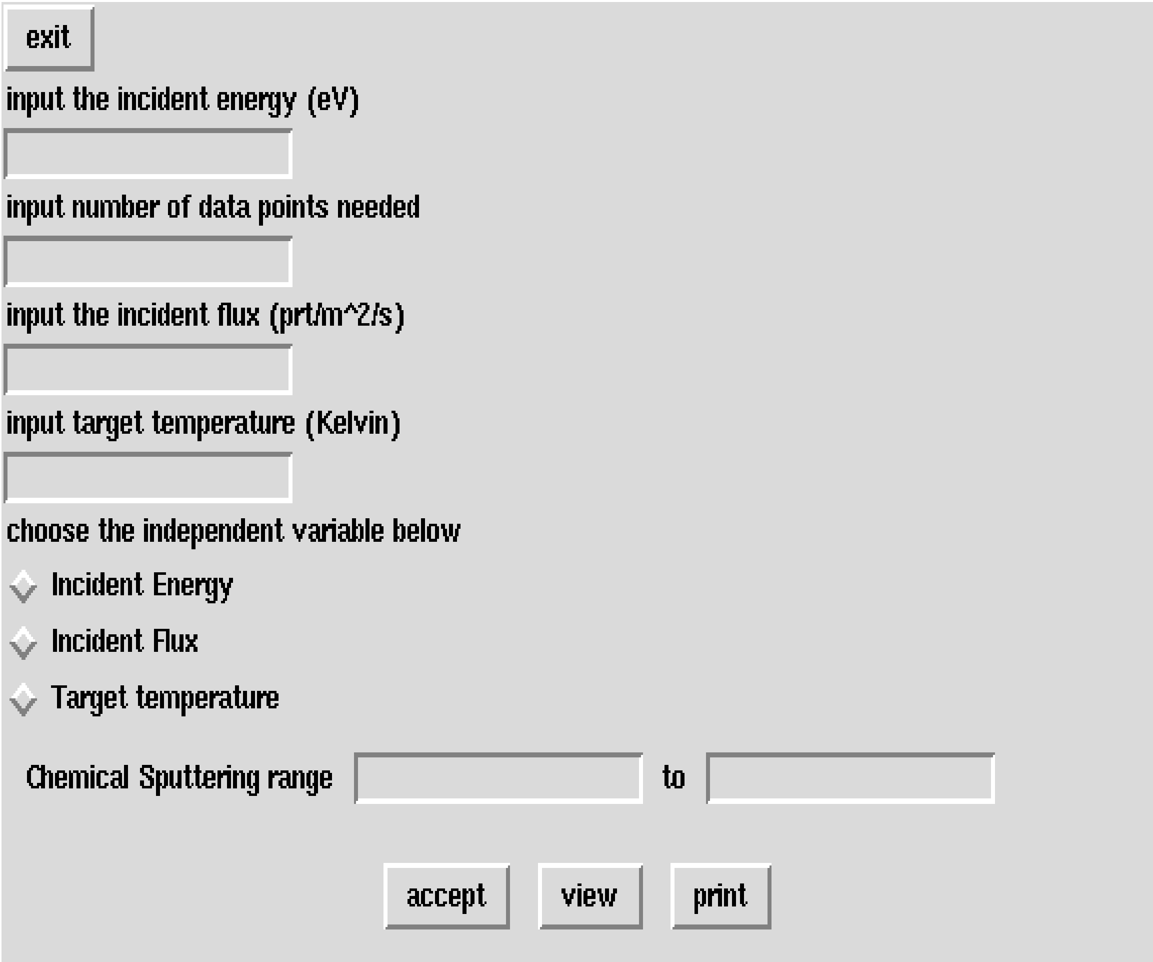

Figure 15: Window for RES

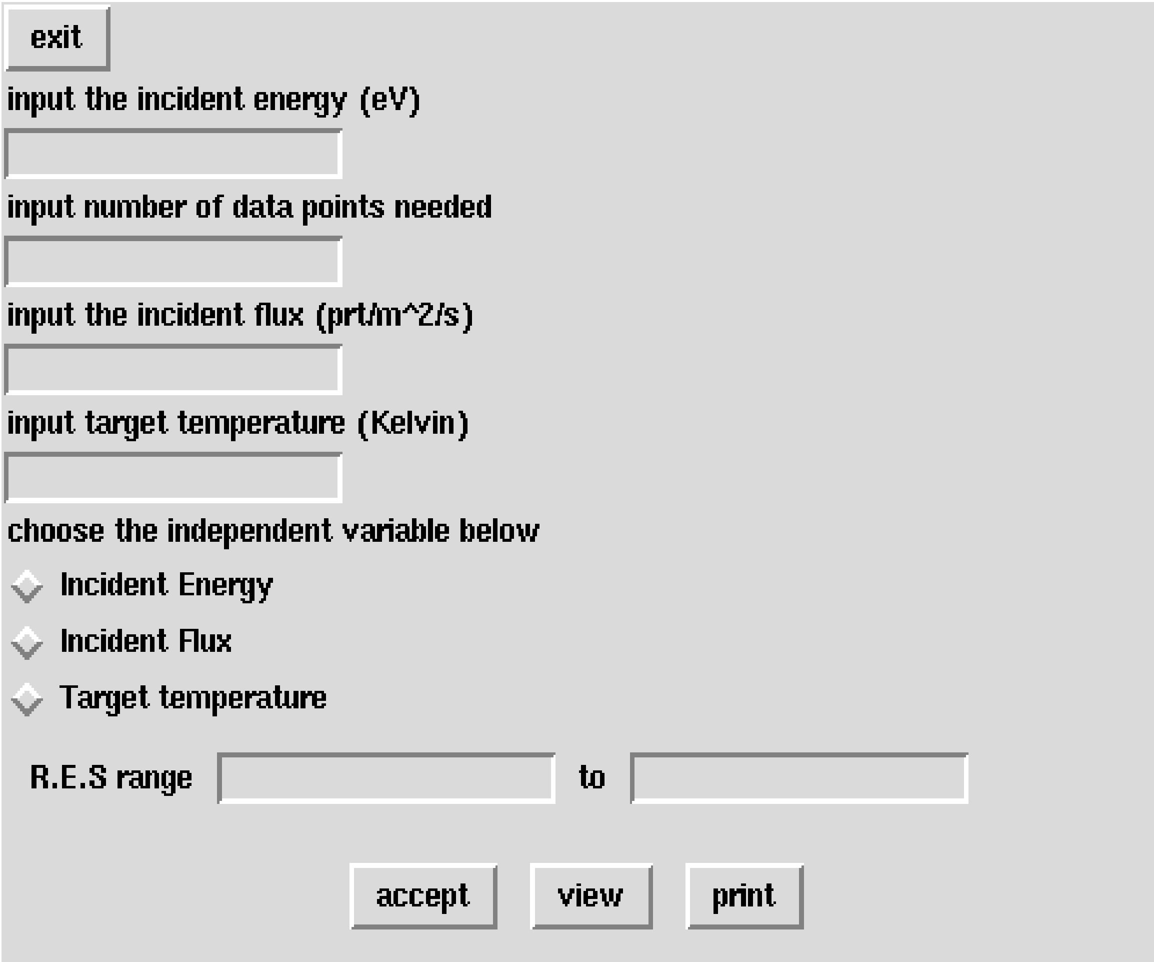

Figure 16: Simplified model of target erosion in a glow discharge

Simple 0-D model for EROSION

Sheath :

$$\underbrace{\frac{3}{2}T_i}_{\text{thermal}} + \underbrace{\frac{1}{2}(T_e + T_i)}_{\text{pre-sheath}} + \underbrace{V}_{\text{sheath}}$$