# The TRIM code surface database

Most of the material in this section has been taken from the report [1].

**Version: 01-2010**

# Contents

# 1 General remarks

For details concerning the physical model, the basic assumptions and the TRIM-code, which was used to generate the data discussed here, we refer to the monograph by W.Eckstein, [2]. For a description of the format of the database, and the random sampling procedure, which allows one to generate the distribution of reflected particles from the data given here, we refer the reader to the earlier works [3] and [4] on the same issue. Whereas in Ref. [3] the data are based upon MARLOWE code calculations, they have been obtained using the TRIM Monte Carlo code in Ref. [4] and in this current database.
The TRIM code assumes an amorphous target, while in the earlier MARLOWE code calculations a crystal target structure was retained. In the TRIM code, the "krypton-carbon potential" was used, whereas in MARLOWE usually the "Moliere potential" was employed. The MARLOWE data in [3] had been produced on the basis of 20,000 particle histories for each incident energy and angle. The TRIM calculations have been performed with 200,000 cascades for each such incident beam, both in Ref. [4] and in this current database. Thus the statistical significance of the more recent TRIM data can be expected to be better, but the trends should be similar as with the MARLOWE code data.
The only difference of this present data compilation to the one presented in [4] is the extension to a larger set of target-projectile combinations here. However, for comparisons and completeness, we have kept the data and the plots for particle, energy and momentum reflection coefficients also for the previous data.
The full database can be found under "downloads". Graphical presentation of some moments derived from that database are available under "Surface Data/Incident Species/Target-Projectile Combination". The definition of these moments is given in the three subsections below.

## 1.1 Particle reflection coefficient

Let $f(E, \theta, \phi \mid E_0, \theta_0) \sin(\theta) dE d\theta d\phi$ denote the probability of reflection of an incident particle with energy $E_0$ and incident polar angle $\theta_0$ against the surface normal, with energy $E$ and into the solid angle $\Omega d\Omega$ with $d\Omega = \sin(\theta) d\theta d\phi$.
Hence: $f$ is, up to normalization, a conditional (on $E_0$ and $\theta_0$) distribution for the energy $E$ and angle $(\theta, \phi)$ of the reflected particle. The azimuthal angle $\phi$ is measured against the incident velocity, i.e. $\phi_0 = 0$.
The "Particle Reflection Coefficient" $R_N$ is the probability of reflection:

$$R_N(E_0, \theta_0) = \int_0^{E_0} \int_0^{\pi} \int_0^{2\pi} dE d\theta d\phi \sin(\theta) f(E, \theta, \phi \mid E_0, \theta_0) \tag{1}$$

$R_N$ is the last number in the first line of the data tables (see: "downloads", and Figure below, in Section 4), i.e. given for each incident $E_0$ and $\theta_0$.
With the normalization

$$\tilde{f} = \frac{1}{R_N} \cdot f \tag{2}$$

$$= \tilde{f}_1(E) \cdot \tilde{f}_2(\theta \mid E) \cdot \tilde{f}_3(\phi \mid E, \theta) \tag{3}$$

one obtains a multivariate probability density $\tilde{f}$ for the velocity space coordinates of the reflected particle, for each given $E_0$ and $\theta_0$.

## 1.2 Energy reflection coefficient

The energy reflection coefficient is defined as

$$R_E(E_0,\theta_0) = \frac{1}{E_0}\int_0^{E_0}\int_0^{\pi}\int_0^{2\pi} dE d\theta d\phi\ \sin(\theta)\ E\ f(E,\theta,\phi \mid E_0,\theta_0) \tag{4}$$

$$= \frac{R_N}{E_0}\int_0^{E_0} dE\ E\ \tilde{f}_1(E \mid E_0,\theta_0) = R_N\frac{\overline{E}_{ref}}{E_0} \tag{5}$$

i.e., as $R_N$ times the ratio of the mean energy of the reflected particle to the incident energy $E_0$.
The second row of the data files, i.e., one row for each fixed $E_0$ and $\theta_0$, contains five numbers (quantiles) $E_1, E_3, E_5, E_7, E_9$ which are defined by the relation:

$$P\{E < E_i\} = Q_i, \text{ with } \quad Q_i = 0.1, 0.3, 0.5, 0.7, 0.9 \tag{6}$$

with $P\{E < E_i\}$ denoting the (cumulative) probability that the energy of the reflected particle is not larger than $E_i$.
Hence, by construction, each of the 5 energies $E_i$ of reflected particles has the same probability $p = 0.2$. The mean energy $\overline{E}_{ref}$ of reflected particles is therefore simply:

$$\overline{E}_{ref} = \overline{E}_{ref}(E_0,\theta_0) = \frac{1}{5}\sum_{i=1}^{5} E_i \tag{7}$$

## 1.3 Momentum reflection coefficient

The (parallel) momentum reflection coefficient is analogously defined as

$$R_M(E_0,\theta_0) = \frac{1}{M_{0,\parallel}}\int_0^{E_0}\int_0^{\pi}\int_0^{2\pi} dE d\theta d\phi\ \sin(\theta)\ M_{\parallel}\ f(E,\theta,\phi \mid E_0,\theta_0) \tag{8}$$

$$= \frac{R_N}{M_{0,\parallel}}\int_0^{E_0} dE\ M_{\parallel}\ \tilde{f}_1(E \mid E_0,\theta_0) = R_N\frac{\overline{M}_{ref,\parallel}}{M_{0,\parallel}} = R_N\frac{\overline{v_{ref,\parallel}}}{v_{0,\parallel}} \tag{9}$$

i.e., as $R_N$ times the ratio of the mean (parallel) momentum $M_{\parallel}$ of the reflected particle to the incident (parallel) momentum $M_{0,\parallel}$.
The incident velocity $\vec{v}_0$ is defined as

$$\vec{v}_0 = (v_{0,\perp}, v_{0,\parallel}, 0) = (v_0\cos\theta_0, v_0\sin\theta_0, 0) \tag{10}$$

with $v_\perp$ and $v_\parallel$ denoting the velocity components normal and parallel to the surface, respectively, $v_0 = \sqrt{2E_0/m}$, with $m$ being the mass of the incident particle.
The velocity of the reflected particle is given as

$$\vec{v}_{ref} = (v_{ref,\perp}, v_{ref,\parallel}, v_{ref,\top}) = (v_{ref}\cos\theta, v_{ref}\sin\theta\cos\phi, v_{ref}\sin\theta\sin\phi) \tag{11}$$

The next block of 5 rows of the data files, i.e., one such block for each fixed $E_0$ and $\theta_0$, contains 25 numbers (quantiles), 5 numbers in each row $i$, $\theta_1^i, \theta_3^i, \theta_5^i, \theta_7^i, \theta_9^i$ which are defined by the relation:

$$P\{\cos\theta < \cos(\theta_j^i) | E_i\} = Q_j^i, \text{ with } \quad Q_j^i = 0.1, 0.3, 0.5, 0.7, 0.9 \tag{12}$$

Hence, by construction, for each given energy of the reflected particle $E_i$, each of the 5 polar angles $\cos(\theta_j^i)$ of the reflected particles has the same probability $p = 0.2$.
Analogously, there are then 5 blocks, each block with 5 rows, each row with 5 numbers, for the quantiles of the conditional distribution of the cosines of azimuthal angles $\phi$. The $i^{th}$ block corresponds to given energy $E_{0,i}$, and the $j^{th}$ row in block $i$ contains these 5 quantiles for given $E_i$ and $\theta_j$:

$$P\{\cos\phi < \cos(\phi_k^{i,j})|E_i, \theta_j\} = Q_k^{i,j}, \text{ with } \quad Q_k^{i,j} = 0.1, 0.3, 0.5, 0.7, 0.9 \tag{13}$$

Hence, again by construction, the mean parallel velocity $\overline{v}_{ref,\parallel}$ of reflected particles, given that the reflected energy is $E_i$ and that the polar angle of reflection is $\theta_j$ is therefore simply:

$$\overline{v}_{ref,\parallel}^{i,j} = \frac{1}{5}\sum_{i=1}^{5} v_{ref}^i \sin(\theta_j^i)\cos(\phi_k^{i,j}) \tag{14}$$

with $v_{ref}^i = \sqrt{2E_i/m}$.
Since all the 5 polar angles $\theta_j^i$ also have same probability $p = 0.2$ by construction (Eq. 12), we can average this over polar angles to obtain for the mean reflected parallel velocity, given that $E_{ref} = E_i$:

$$\overline{v}_{ref,\parallel}^{i} = \frac{1}{5}\sum_{j=1}^{5} \overline{v}_{ref,\parallel}^{i,j} = \frac{1}{25}\sum_{j=1}^{5}\sum_{k=1}^{5} v_{ref}^i \sin(\theta_j^i)\cos(\phi_k^{i,j}) \tag{15}$$

and, finally, averaging over the 5 energies $E_i$ (all have the same probability $p = 0.2$), we find

$$\overline{v}_{ref,\parallel} = \frac{1}{5}\sum_{j=1}^{5} \overline{v}_{ref,\parallel}^{i} = \frac{1}{125}\sum_{i=1}^{5}\sum_{j=1}^{5}\sum_{k=1}^{5} v_{ref}^i \sin(\theta_j^i)\cos(\phi_k^{i,j}) \tag{16}$$

Hence, $R_M$ can be evaluated from each table, i.e. for each target-projectile combination and for each incident energy $E_0$ and angle $\theta_0$. Of course, for normal incidence ($\theta_0 = 0$) also $v_{0,\parallel} = 0$ , Eq. (10). In this case $R_M$ is not defined and set to zero.

# 2 Target-projectile combinations

The databases had been set up in references [3] and [4] for the following target-projectile combinations:

D onto Fe (Ref. [3], MARLOWE code, "Histogram quantile estimator")
T onto Fe (ditto)
He onto Fe (ditto)
(This database is available upon request, but not in use anymore in the EIRENE Monte Carlo code package)

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H onto Fe and H onto C (Ref. [4], TRIM code, "Histogram quantile estimator")
D onto Fe and D onto C (ditto)

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We have, until June 2001, added the following combinations:

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H onto Cu , H onto Mo and H onto W (TRIM Code)
D onto Mo, D onto W and D onto Be (ditto)
T onto Fe, T onto C, T onto Mo and T onto W (ditto)
He onto Fe, He onto C, He onto W and He onto Mo (ditto)
Ne onto C, and Ne onto Be (ditto)

(Further updates: see below: section 6)

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# 3 The input data

The TRIM code version used here is **NEWTRD**, which is a static vectorized version for reflection off a one-component target.
Some of the physical input parameters which have been specified for the TRIM code calculations for these particular combinations are listed in the table below. A detailed description of the physical model is given in [2]. The short description given below is from W.Eckstein, IPP Garching, April 1991, private communication.

The input data file consists of 4 cards:

```
Z1   M1   Z2  M2    RHO  TT    ED
E0   EF   X0  ALPHA CK   CA    CW
NH   RI   ESB KDEE  KK0  INEL  DGI
H1   H2   H3  H4    H5
```

First card:

- **Z1** atomic number of projectile
- **M1** mass (in amu) of projectile
- **Z2** atomic number of target atom
- **M2** mass (in amu) of target atom
- **RHO** target density ( in g/cm**3)

  The reflection coefficients should be independent of **RHO**.
- **TT** target thickness ( in Å)
- **ED** displacement energy (in eV)

  Not relevant for sputtering or reflection as used here, but only for radiation damage calculations.

Second card

- **E0** energy of projectile (in eV)
- **EF** cutoff energy of projectiles (in eV)
  must be larger than zero
- **X0** starting depth of projectile (in Å)
  If x0 is zero or negative the projectile starts at $x = -su = -2. \cdot pmax$. The uppermost target atoms are at x=0. They do not form a complete layer, they are distributed randomly.
- **ALPHA** angle of incidence (in degree) with respect to surface normal
- **CK** correction factor to the Lindhard-Scharff nonlocal inelastic energy loss of the projectile

- **CA** correction factor to the Firsov screening length for collisions between projectile and target atom (only for application of Moliere-potential)
- **CW** depth interval for calculated depth distribution (in Å)

  Not relevant for sputtering or reflection as used here, but only for depth profile evaluation. In this latter case reasonable choices for **CW** depend also on incident energy and angle.

Third card

- **NH** number of test projectiles (Monte Carlo histories)
- **RI** initial random number
- **ESB** surface binding energy for projectiles (in eV)
- **KDEE** inelastic energy loss model for projectiles
  - = 1 nonlocal, Lindhard-Scharff
  - = 2 local, Oen-Robinson
  - = 3 equipartition of 1 and 2
  - = 4 nonlocal, Andersen-Ziegler tables for hydrogen,
    for energies larger than 20 keV, i.e. irrelevant for present database.
  - = 5 nonlocal, Ziegler tables for helium,
    for energies larger than 80 keV, i.e. irrelevant for present database.
- **KK0** maximum order of weak (simultaneous) collisions between projectiles and target atoms. KK0 must be between 0 and 4 (4 means: no weak collisions included)
- **INEL** inelastic energy loss outside the surface
  $= 0$: no inelastic energy loss outside the target
  $\neq 0$: see hlm (below)
- **DGI** angular interval of the azimuthal angle for matrices

Fourth card

- **H1,. . . ,H5** constants for the nonlocal inelastic energy loss given by Andersen-Ziegler tables for hydrogen or by Ziegler tables for helium. See remarks for **KDEE** flag above. I.e., these parameters are irrelevant for present database.

**Fixed parameters for all cases documented here:**

- **TT** =99000.
- **X0** =0.0
- **CK** =1.0
- **CA** =1.0

- **NH** =200000
- **RI** =29303.0
- **KDEE** =3
- **DGI** =30.0
- **H1** =4.652
- **H2** =0.4571
- **H3** =80.73
- **H4** =22.0
- **H5** =4.952

**Fixed Parameters for all Be targets**

- **Z2** =4
- **M2** =9.012
- **RHO** =1.85 (also in use: **RHO**=1.80)

**Fixed Parameters for all C targets**

- **Z2** =6
- **M2** =12.01
- **RHO** =2.26 (for graphite used in fusion often also: **RHO**=1.85)

**Fixed Parameters for all Fe targets**

- **Z2** =26
- **M2** =55.85
- **RHO** =7.87

**Fixed Parameters for all W targets**

- **Z2** =74
- **M2** =183.85
- **RHO** =19.30

## 3.1 Hydrogen projectiles

**Fixed Parameters for all H - projectile cases**

- **Z1** =1
- **M1** =1.01
- **ESB** =1.0

| | Hydrogen Projectiles onto: | | | | | |
|---|---|---|---|---|---|---|
| | Be | C | Fe | Cu | Mo | W |
| Ref. | Knauf | Eckstein | Eckstein | ? | ? | Knauf |
| ED | ? | 25 | 17 | 19 | 33 | 35.0 ? |
| EF | ? | 0.95 | 0.95 | ? | ? | 0.95 |
| CW | ? | 5 | 5 | ? | ? | 10.0 |
| KK0 | ? | 2 | 2 | 2 | 2 | 3 |

## 3.2 Deuteron projectiles

**Fixed Parameters for all D - projectile cases**

- **Z1** =1
- **M1** =2.01
- **ESB** =1.0

| | Deuteron Projectiles onto: | | | | |
|---|---|---|---|---|---|
| | Be | C | Fe | Mo | W |
| Ref. | Knauf | Eckstein | Eckstein | ? | Knauf |
| ED | ? | 25 | 17.0 | 33 | 35.0 ? |
| EF | 0.98 | 0.95 | 0.98 | ? | 0.95 |
| CW | 4.0 | 5.0 | 4.0 | ? | 10.0 |
| KK0 | 2 | 2 | 3 | ? | 3 |

## 3.3 Triton projectiles

**Fixed Parameters for all T - projectile cases**

- **Z1** =1
- **M1** =3.02
- **ESB** =1.0

| | Triton Projectiles onto: | | | | |
|---|---|---|---|---|---|
| | Be | C | Fe | Mo | W |
| Ref. | ? | Reiter | Reiter | ? | Reiter |
| ED | ? | 25.0 | 17.0 | 33 | 38 |
| EF | ? | 0.98 | 0.98 | ? | 0.95 |
| CW | ? | 4.0 | 4.0 | ? | 5 |
| KK0 | ? | 2 | 2 | ? | 3 |

## 3.4 Helium projectiles

**Fixed Parameters for all He - projectile cases**

- **Z1** =2
- **M1** =4.00
- **ESB** =0.0

| | Helium Projectiles onto: | | | | |
|---|---|---|---|---|---|
| | Be | C | Fe | Mo | W |
| Ref. | ? | Reiter | Reiter | ? | Eckstein |
| ED | ? | 25.0 | 17.0 | 33 | 35 |
| EF | ? | 0.20 | 0.20 | ? | 0.10 |
| CW | ? | 10.0 | 3.0 | ? | 10.0 |
| KK0 | ? | 2 | 2 | ? | 2 |

## 3.5 Neon projectiles

**Fixed Parameters for all Ne - projectile cases**

- **Z1** =10
- **M1** =20.183
- **ESB** =0.0

| | Neon Projectiles onto: | | | | |
|---|---|---|---|---|---|
| | Be | C | Fe | Mo | W |
| Ref. | ? | Knauf | ? | ? | Eckstein |
| ED | ? | 25.0 | 17 | 33 | 38 |
| EF | ? | 0.20 | ? | ? | 0.5 |
| CW | ? | 10.0 | ? | ? | 5 |
| KK0 | ? | 2 | ? | ? | 2 |

# 4 Data format, and random sampling

Distribution functions for back-scattered particles are available for incident energies of 1, 2, 5, 10, 20, 50, 100, 200, ..., 5000 eV, and for incident polar angles of 0, 30, 45, 60, 80 and 85 degrees against the surface normal.
The distribution function for back-scattered particles in velocity space is represented by tables of conditional quantile functions, as explained in [3] (although this statistical terminology is not mentioned explicitly there). Each such table corresponds to one particular target projectile combination, one particular incident energy and one particular incident polar angle. Hence there are $84\ (= 12 \cdot 7)$ tables for each target projectile combination.
In the first line of each table the nuclear mass and charge numbers of target and projectile, respectively, are given, followed by incident energy (eV) and angle (degrees) and the particle reflection coefficient.
The next line is a list of 5 numbers for the backscattered energy distribution (corresponding to the 5 energy values, which belong to the 5 (uniformly distributed) random numbers 0.1, 0.3, 0.5, 0.7 and 0.9). Next there is a table of 25 numbers for the cosine of the polar emission angle (5 rows of 5 numbers each). Each row corresponds to one of the five energy values from the previously mentioned energy distribution. Within each row (i.e., for fixed backscattered energy) the values correspond to the 5 polar angles, which correspond to the 5 uniformly distributed random numbers 0.1, 0.3, 0.5, 0.7, 0.9 .
Finally there is a block of 125 numbers for the azimuthal distribution, 5 blocks consisting of 5 rows of 5 numbers each. The choice of a block is made with the same random number as used for the energy, the row number within one block is selected using the second (polar angle) random number, and the column in this row is determined then by a third random number.
The full database for one particular target - projectile combination consists of 84 such tables (12 incident energies and 7 incident polar angles).
Use of these tables has been explained in [5] and [4]. However, unfortunately the examples for the one particular triple of random numbers given in these references [5] and [4] are wrong. A projectile-target case: D on Fe was chosen. For the three random numbers $\xi_1 = 0.3, \xi_2 = 0.5$ and $\xi_3 = 0.9$ and for an incident energy of 200 eV and an incident polar angle of 30 degrees as chosen in [5], the sampled energy of the reflected particle should be 91.665 eV (as correctly stated in [5]) but for the polar and azimuthal angles $\theta$ and $\phi$ one must find $\cos\theta = 0.778114$ and $\cos\phi = 0.942824$ in this case, distinct from the values given in the references by Heifetz and Eckstein.
The same triple of random numbers, for example, applied to the table for helium onto carbon, 200 eV, normal incidence, would yield: $26.905$ eV, $\cos\theta = 0.83113$ and $\cos\phi = 0.94738$.
The correct interpretation of the data can be easily checked, e.g., by using the fact that for the tables corresponding to normal incidence, the resulting azimuthal distribution must be isotropic. Note that, e.g. in the faulty example in Ref. [5] and [4], this is not the case.
The EIRENE code uses these tables, for a continuous spectrum of incident energies and angles, as well as for a continuous triple of independent, uniformly distributed random numbers by multiple linear interpolation in the tables.

D --> Fe

| | | | $E_{in}$ | $\vartheta_{in}$ | $R_N$ | |
|---|---|---|---|---|---|---|
| | | $E_2$ | | | | |
| 1. | 2.00 | 26. | 56.00 | 2.00E+02 | 3.00E+01 | 4.80E-01 |

| | | | | | |
|---|---|---|---|---|---|
| 4.11620E+01 | 9.16650E+01 | 1.25390E+02 | 1.50840E+02 | 1.72260E+02 | — $E_i$ , i=1,5 |
| | | | cos $\vartheta_3^2$ | | |
| 4.82510E-01 | 6.71020E-01 | 7.93260E-01 | 8.86500E-01 | 9.64970E-01 | |
| 4.64730E-01 | 6.53370E-01 | 7.78110E-01 | 8.76670E-01 | 9.60970E-01 | |
| 4.33170E-01 | 6.27780E-01 | 7.58580E-01 | 8.67410E-01 | 9.57180E-01 | cos $\vartheta_j^i$ |
| 4.18910E-01 | 6.07690E-01 | 7.37670E-01 | 8.49380E-01 | 9.52100E-01 | |
| 3.16180E-01 | 4.77130E-01 | 6.08050E-01 | 7.38090E-01 | 8.90090E-01 | |
| | | | cos $\varphi_5^{2,3}$ | | |
| -9.40740E-01 | -5.56890E-01 | 6.39960E-02 | 6.32580E-01 | 9.56660E-01 | |
| -9.43650E-01 | -5.83060E-01 | -2.24480E-02 | 5.53250E-01 | 9.38340E-01 | |
| -9.42090E-01 | -5.90000E-01 | -3.12500E-02 | 5.86500E-01 | 9.51360E-01 | i=1 |
| -9.48140E-01 | -5.63720E-01 | 3.37290E-03 | 6.00100E-01 | 9.56280E-01 | |
| -9.48830E-01 | -5.67360E-01 | -1.34340E-02 | 5.95890E-01 | 9.56690E-01 | |
| -9.39810E-01 | -5.87230E-01 | -2.29360E-02 | 5.59450E-01 | 9.44810E-01 | |
| -9.54800E-01 | -5.73700E-01 | 3.88110E-02 | 5.87850E-01 | 9.49180E-01 | |
| -9.45890E-01 | -5.85990E-01 | -4.72020E-02 | 5.59330E-01 | 9.42820E-01 | i=2 |
| -9.46810E-01 | -6.23760E-01 | -4.98030E-02 | 5.61960E-01 | 9.39650E-01 | |
| -9.52460E-01 | -5.42690E-01 | 5.07270E-02 | 6.15900E-01 | 9.60990E-01 | |
| -9.45580E-01 | -5.56640E-01 | 2.38740E-02 | 6.11950E-01 | 9.62670E-01 | |
| -9.42630E-01 | -5.42540E-01 | 3.99670E-02 | 6.07410E-01 | 9.51140E-01 | |
| -9.52150E-01 | -5.53460E-01 | 4.96280E-02 | 6.20170E-01 | 9.55360E-01 | i=3 |
| -9.36370E-01 | -5.59120E-01 | 2.80660E-02 | 6.24860E-01 | 9.44440E-01 | |
| -9.48420E-01 | -5.61020E-01 | 3.99420E-03 | 5.94790E-01 | 9.49920E-01 | |
| -9.35360E-01 | -4.59090E-01 | 1.55120E-01 | 6.70960E-01 | 9.52260E-01 | |
| -9.36900E-01 | -4.98860E-01 | 1.52800E-01 | 6.60320E-01 | 9.60450E-01 | |
| -9.37110E-01 | -5.15800E-01 | 1.07910E-01 | 6.31570E-01 | 9.61270E-01 | i=4 |
| -9.35620E-01 | -5.13910E-01 | 1.37290E-01 | 6.88520E-01 | 9.63320E-01 | |
| -9.43480E-01 | -5.41080E-01 | 7.34930E-02 | 6.16980E-01 | 9.47230E-01 | |
| -7.03640E-01 | -2.60170E-02 | 4.62110E-01 | 8.07130E-01 | 9.81170E-01 | |
| -6.50590E-01 | -7.77770E-04 | 5.20590E-01 | 8.27840E-01 | 9.80430E-01 | |
| -6.36710E-01 | -3.04950E-02 | 4.52520E-01 | 7.94420E-01 | 9.75290E-01 | i=5 |
| -6.26120E-01 | -5.22300E-02 | 4.84880E-01 | 8.20230E-01 | 9.78380E-01 | |
| -5.59810E-01 | -7.71550E-02 | 3.96120E-01 | 7.88740E-01 | 9.76690E-01 | |

cos $\varphi_k^{ij}$

Figure 1: Sample reflection data table, for D on Fe, 200 eV, 30 degrees incident energy and angle, respectively. Marked are the reflection energy, polar and azimuthal angles for the triple of random number (0.3, 0.5, 0.9)

# 5 Scaling to other target – projectile combinations

In case a particular target (B) projectile (A) data file `A_on_B` is not available in an EIRENE run, then the following reduced energy scaling procedure is applied:
Let $A$ be the incident particle, with energy $E$, mass $m_A$, nuclear charge $Z_A$ and let $B$ be the stationary ($E_B = 0$) target, characterized by $m_B, Z_B$. Then the reduced energy $\epsilon_{A,B}$ is defined as:

$$\epsilon_{A,B} = E/E_{TF} = E_r/C = E_r/\left(\frac{Z_A Z_B e^2}{a}\right) \tag{17}$$

with $E_r$ the center of mass collision energy: $E_r = E \cdot m_B/(m_A + m_B)$, $e$ the elementary charge: $e^2 = 14.39$ eV Å and $a$ is the *Thomas Fermi screening length* (also: *Lindhard screening length*):
$a = 0.4685(Z_A^{2/3} + Z_B^{2/3})^{-1/2}$ Å.

The energy $E_{TF}$

$$E_{TF} = 30.74 \frac{m_A + m_B}{m_B} Z_A Z_B (Z_A^{2/3} + Z_B^{2/3})^{1/2}$$

implicitly defined by the above relation is the so called Thomas Fermi energy, a parameter that appears in a natural way when reflection (and physical sputtering) is predominantly determined by the nuclear stopping cross section.
$\epsilon_{A,B}$ is a universal dimensionless energy, resulting from the binary collision approximation and elastic collision kinetics, and this reduced energy often allows a unified presentation of surface reflection data vs. energy for different target projectile combinations, see for example [2].
The procedure in an EIRENE run is now as follows:
Given a particle of species $A$ has hit a surface of material $B$. If the surface reflection data file `TRIM-A_on_B` is available in a particular EIRENE run, then this data file is used to determine the reflection probability, energy and angles.
If this file is not active in a particular run (e.g.: if it was not selected in the input file, or if this particular target-projectile combination is not available in the EIRENE surface database at all), then EIRENE computes the Thomas Fermi energies $E_{TF}(A_i, B_i)$ for all target-projectile combinations $A_i, B_i$, for which it does have such TRIM data files. It then identifies amongst those the one $A_{i'}, B_{i'}$ for which the ratio

$$E_{TF}(A, B)/E_{TF}(A_{i'}, B_{i'}) = \epsilon_{A,B}/\epsilon_{A_{i'},B_{i'}} =: f_{reduc}^{-1}$$

is closest to one. The target projectile combination selected in this way can hence be regarded as being "physically most similar" to the system `A_on_B`. EIRENE then changes the incident energy $E$ to $\tilde{E} = E \cdot f_{reduc} = E \cdot \epsilon_{A_{i'},B_{i'}}/\epsilon_{A,B}$ and then carries out its surface reflection procedure according to TRIM model $A_{i'}, B_{i'}$ for incident energy $\tilde{E}$. The energy $\tilde{E}_{ref}$ of the reflected particle is then finally scaled back to the `A_on_B` system by the relation $E_{ref} == \tilde{E}_{ref}/f_{reduc} = \tilde{E}_{ref} \cdot \epsilon_{A,B}/\epsilon_{A_{i'},B_{i'}}$.
Note that due to the wide range of available TRIM data files in the EIRENE database the scaling factors turn out to be close to one, typically, and this entire procedure can therefore be regarded as being a quite robust interpolation scheme in the TRIM database.
Finally we note that in case of physical sputtering a similar reduced energy scaling can be carried out, because the same Thomas Fermi energy also appears in theoretical treatments of sputtering. But strictly this scaling is justified only for the high energy region $E \gg E_{th}$ with $E_{th}$ denoting the finite threshold energy. A generalized "reduced energy scaling for sputtering", involving both controlling parameters $E_{TF}$ and $E_{th}$, and hence accounting for the different scaling near the important threshold energy for the sputtering process, has been given e.g. in [7].

# 6 Updates

The TRIM surface reflection database has been updated in 2007 by a number of further target-projectile combinations, obtained from S. Droste, FZ-Juelich, see:

Stefan Droste, "Simulation von Erosions- und Depositionsprozessen mehrkomponentiger Oberflächenschichten in Fusionsanlagen", Report Jül-4253, August 2007, ISSN 0944-2952

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