

SRIM Textbook

SRIM *The Stopping and Range* *of Ions in Matter*

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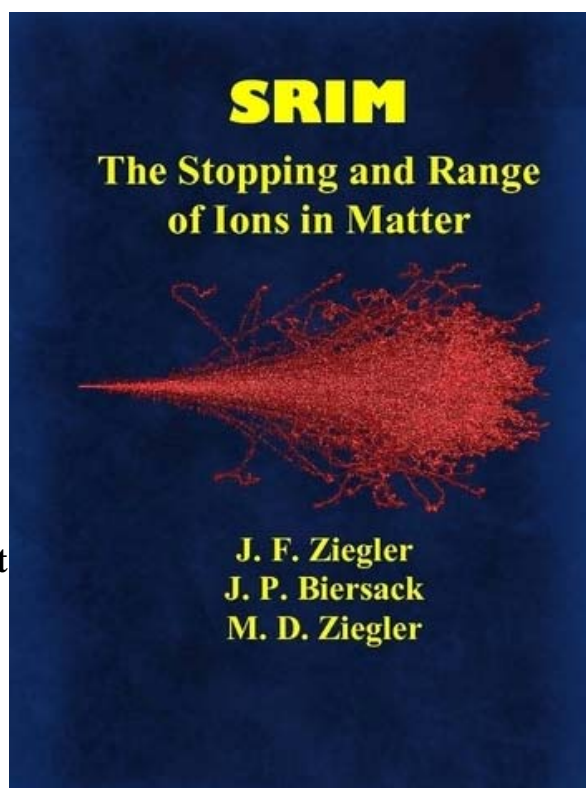
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The SRIM textbook covers the physical phenomena associated with the penetration of energetic ions into matter. It is primarily concerned with the quantitative evaluation of how ions lose energy into matter and the final distribution of these ions after they stop within the target. Also considered are the first order effects of the atoms on solids, particularly the electronic excitation of the atoms, the displacement of lattice atoms by energetic collisions (lattice damage) and the production of plasmons and phonons within the solid by the passing ions. No evaluation is made of thermal effects in the solid, especially redistribution of lattice atoms or implanted ions by thermal or vacancy induced diffusions.

The scientific literature contains a large amount of experimentally determined stopping powers and ion range distributions. These are not, however, so accurate or dense that direct interpolation to other systems is usually possible. The main goal of this work is to establish methods for determining the stopping and range of ions based on accurate experimental data and extending these values using unified theoretical concepts.

SECT. 2 THE TRIM CODE

Ref: J. F. Ziegler, J. P. Biersack and U. Littmark, *The Stopping and Range of Ions in Matter*,

- TRIM(TRANsport of Ions in Matter) calculates all interactions of a *projectile*(ion or a neutral atom) with a solid consisting of stationary *target* atoms.
- TRIM is part of a code package SRIM, which can be downloaded from the web at www.SRIM.org
- The code is basically a Monte Carlo calculation. One projectile at a time is incident on the solid surface. The trajectories of the projectile and the recoil target atoms are followed.
- TRIM is user-oriented, unlike the research codes described in Sect. 1

The input information required for the calculation includes:

- projectile: Z_1 , M_1 , of the initial energy E_{i0}
- target: Z_2 , M_2 , thickness and density
- The displacement energy of the atoms in the target materials(E_d).
- The surface atom binding energy(for sputtering calculations).
- Binding energy of lattice (target) atoms, E_b

The output of the computation includes:

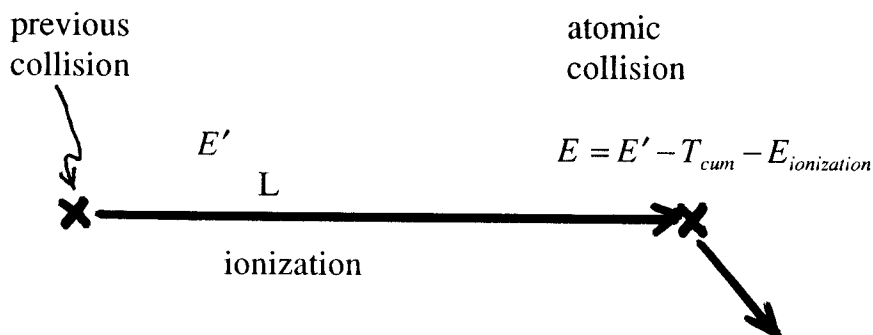
- The path of the projectile and of all recoil target atoms
- The depth distribution of the atomic displacements(dpa) of the target atoms
- final position of the projectile(i.e., range and range straggling)
- Projectile energy loss by ionization(electronic stopping); histories of all recoils
- Sputtering of the surface atoms
- Projectile reflection via the front surface or transmission through the rear surface.

Projectile-Medium Interaction Process

- Only two-body collisions are considered
- The computation treats a three-dimensional array of atoms of the solid
- The solid is assumed to be amorphous. Crystal effects(focussing or channeling) and the effect of accumulated damage are not treated
- The target may consist of multiple layers each containing several different elements.

Method of treating the mean free path between atomic collisions (projectile-target or target-target)

- The usual mean free path(the reciprocal of the total cross section times the target atom density) cannot be used because the total cross section for most atomic collisions is infinite(e.g., the Rutherford cross section).
- Instead, a "free-flight distance" L is introduced. This is the distance between large-angle atomic collisions. Rather than trying to calculate the individual effect of the preponderant grazing collisions, only the angular deviation due to these collisions is kept track of. When the angular deviation of the particle under consideration reaches an arbitrary small value, a large-angle collision is permitted to occur. In addition, during the free-flight distance, electronic stopping reduces the energy of the moving atom.



E' = projectile energy at start of flight path

T_{cum} = energy loss due to glancing atomic collisions during flight

$E_{\text{ionization}}$ = ionization loss to electrons of medium during flight Slides 35 – 39

E = projectile energy at point of large-angle nuclear collision.

- At the end of the free-flight path length, an impact parameter for the atomic collision(p) is picked randomly. The method for computing L and p is given later.

- Knowing the energy of the projectile and the impact parameter, the center-of-mass(CM) scattering angle is computed by collision dynamics theory. The projectile or recoil atom loses energy as it proceeds through a series of such free flights and collisions. The process ceases when the energy of the moving atom is too low to cause further displacements(i.e., $< E_d$).

- The detailed histories of recoils and the development of collision cascades are followed in the same manner as described above for the incident ion. Isolated cascade theory(e.g., Eq (55)) is not used since the cascade is determined by following each particle in it individually.

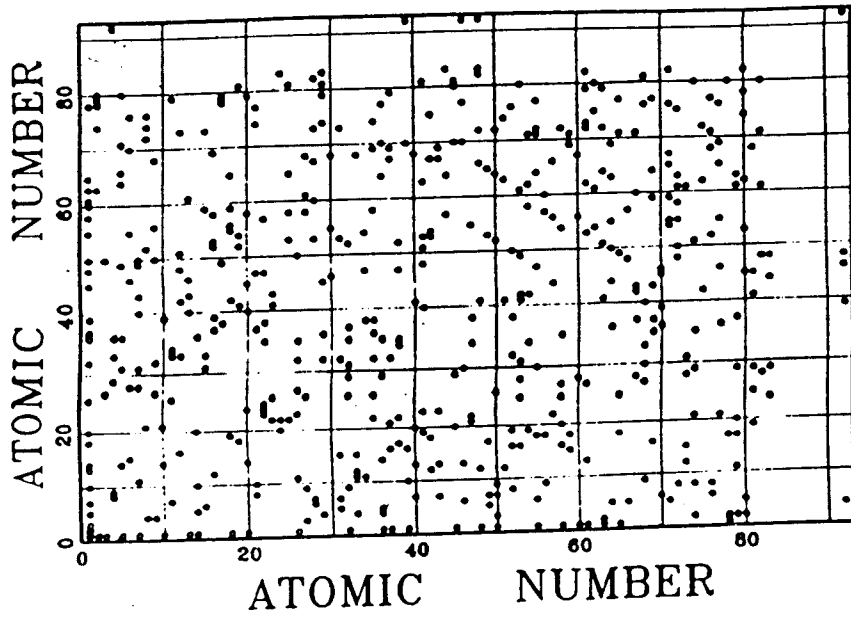
Universal Atomic Potential

- The projectile interacts with atoms of the medium according to interaction laws based on a composite("Universal") interatomic potential that fits a large number of projectile-target atom combinations over a wide range of energies:

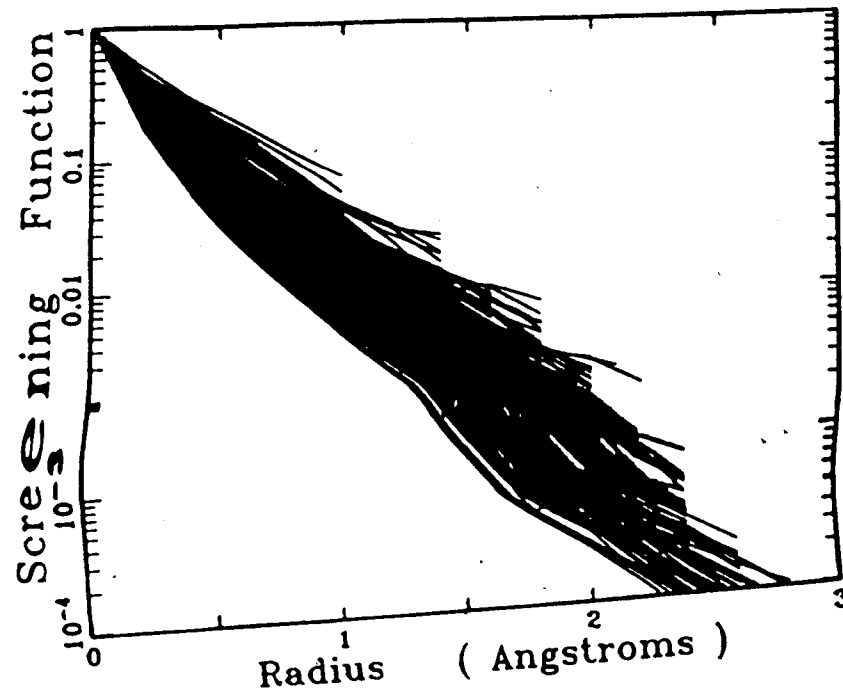
$$V(r) = \frac{Z_1 Z_2 e^2}{r} \Phi\left(\frac{r}{a}\right) \quad (2.1)$$

Φ is a "universal" screening function that has been empirically determined by fitting exact interatomic potentials to Eq(2.1) for a 521 element combinations(out of $\sim 10^4$) over a wide energy range.

Combinations analyzed for the Universal Screening Function



Interatomic Screening Functions for Individual Pairs



The curves are collapsed into the Universal Screening Function using the reduced separation distance r/a :

$$\Phi\left(\frac{r}{a}\right) = \sum_{i=1}^4 A_i \exp\left[-B_i\left(\frac{r}{a}\right)\right] \quad (2.2)$$

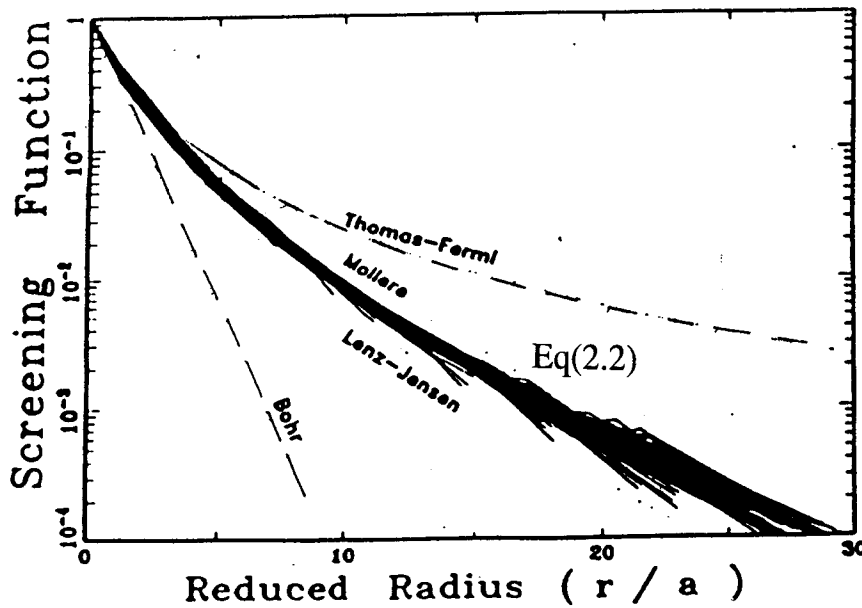
where A_i and B_i are constants that are valid for all elements at all energies.

The parameter a in Eqs(2.1) and (2.2) is an empirical screening length given by:

$$a = \frac{0.8854a_{Bohr}}{Z_1^{0.23} + Z_2^{0.23}} \quad (2.3)$$

$$a_{Bohr} = 0.53 \text{ \AA} = \text{Bohr radius of the hydrogen atom}$$

Universal screening function



- Substitution of Eq(2.1) into the classical scattering integral Eq (32) of Sect. 1

$$\theta = \pi - 2 \int_{r_0}^{\infty} \frac{p dr}{r^2 \left[1 - \frac{V(r)}{E_c} - \frac{p^2}{r^2} \right]^{1/2}} = \pi - 2 \int_{(r_0/a)}^{\infty} \frac{(p/a) dX}{X^2 \left[1 - \frac{1}{X} \frac{\Phi(X)}{\epsilon} - \frac{(p/a)^2}{X^2} \right]^{1/2}} \quad (2.4)$$

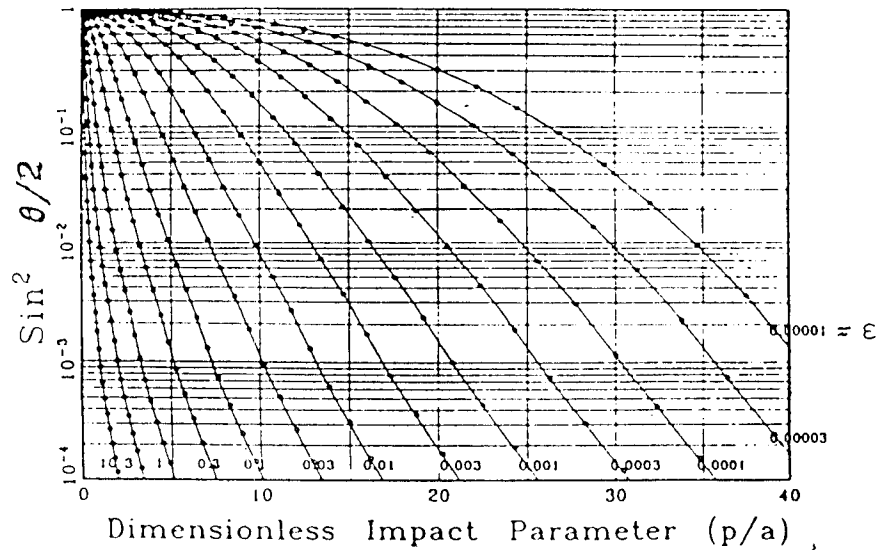
yields the CM scattering angle as a function of the reduced impact parameter p/a and the reduced relative kinetic energy of the collision:

$$\epsilon = \frac{E_c}{(Z_1 Z_2 e^2 / a)} \quad (2.5)$$

where the relative kinetic energy of the projectile or recoil is related to its lab kinetic energy by:

$$E_c = \frac{M_2}{M_1 + M_2} E \quad (2.6)$$

The result is the *Universal Scattering Integral*



Computational algorithm

1. Start with projectile of known energy E (at end of free-flight path)
2. Pick the impact parameter p^*
3. Use the universal scattering integral to determine the CM scattering angle(θ)
 - (a) The projectile scattering angle in the lab frame(Eq(17.11a) of the text) is:

$$\tan \phi = \frac{\sin \theta}{\cos \theta + M_1/M_2} \quad (2.7)$$

- (b) $E' =$ new energy of the projectile = $E - T$, with T from Eq(1.1)
4. $T - E_b$ of recoil; becomes E' for this particle; it is followed along with all of its secondary displacements until $E < E_d$.
5. Find free-flight distance L^*
6. At the end of the free-flight path of any energetic particle, the energy is

$$E = E' - T_{cum} - E_{ionization} \quad (2.8)$$

7. Follow the injected ion until its energy is too low to displace a lattice atom:

$$E_{i,min} = E_d/\Lambda$$

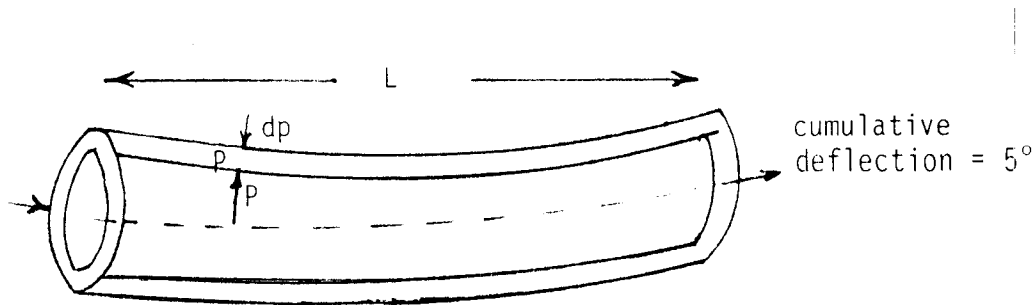
8. Inject another ion at the surface
9. Stop when the statistics are good enough

* The method of determining L and p is described below.

INTERCOLLISION FLIGHT PATH AND IMPACT PARAMETER

High-energy projectile

At high projectile energy, most deflections are small (i.e., less than 1° in the lab system). This is because the dominant contribution to the cross section is due to the Coulomb potential, which produces the forward-peaked Rutherford cross section. TRIM allows many of these small-angle atomic collisions to take place without calculating the details of each one. The large-angle collision is allowed to occur after the cumulative deflection of the projectile by the small-angle collisions reaches 5° . Such a path is shown schematically below.



The free-flight length L is determined as follows. When the angular deflection is small, Eq(2.7) reduces to:

$$\phi = \frac{\theta}{1 + M_1/M_2} \quad (2.9)$$

The energy transferred to the target atom during the collision is:

$$T = \frac{1}{2} \Lambda E (1 - \cos \theta) = \Lambda E \sin^2 \left(\frac{\theta}{2} \right) \quad (2.10)$$

Using Eq(2.9) and simplifying for low-angle collisions yields:

$$\frac{T}{E} = \Lambda \sin^2\left(\frac{\theta}{2}\right) \sim \frac{\Lambda\theta^2}{4} = \frac{\Lambda}{4}\left(1 + \frac{M_1}{M_2}\right)^2 \phi^2$$

but

$$\frac{\Lambda}{4}\left(1 + \frac{M_1}{M_2}\right)^2 = \frac{1}{4} \frac{4M_1M_2}{(M_1+M_2)^2} \frac{(M_1+M_2)^2}{M_2^2} = \frac{M_1}{M_2}$$

Over many small-angle collisions, ϕ is interpreted as the cumulative deflection and T is the sum of the energy losses due to the small-angle atomic collisions that occur over the free-flight path.

$$\phi_{cum} \sim \left(\frac{M_2 T_{cum}}{M_1 E}\right)^{1/2} \quad (2.11)$$

The energy transfer to atoms of the solid due to many glancing atomic collisions can be related to a nuclear(i.e., atomic) stopping power:

$$T_{cum} \sim \left|\frac{dE}{dx}\right|_{nucl} L \quad (2.12)$$

The stopping power is defined by Eq(1.9):

$$\left|\frac{dE}{dx}\right|_{nucl} = N \int_0^{T_{max}} T \sigma(E, T) dT$$

where N is the density of target atoms in the solid. The differential energy-transfer cross section is related to the impact parameter by the analog of Eq(1.27):

$$\sigma(E, T) dT = 2\pi p dp$$

So that with Eq(2.10):

$$\left|\frac{dE}{dx}\right|_{nucl} = N \int_0^{\infty} T 2\pi p dp = 2\pi \Lambda E N \int_0^{p_{max}} \sin^2\left(\frac{\theta}{2}\right) p dp \quad (2.13)$$

In the second integral, the upper limit has been set equal to p_{max} , which is the sum of the atomic radii of the projectile and target atoms. The interatomic potential is essentially zero for larger separation distances.

Substituting Eq (2.13) into (2.12) and then into (2.11) yields:

$$\phi_{\text{cum}}^2 = 2\pi\Lambda LN \frac{M_2}{M_1} \int_0^{p_{\text{max}}} \sin^2\left(\frac{\theta}{2}\right) p dp \quad (2.14)$$

In order to utilize the plot on p. 6, the variable of integration is converted to p/a , where a is the universal screening length (Eq(2.3)). Setting $\phi_{\text{cum}} = 0.09$ radians, the flight path L is given by:

$$L = \frac{(0.09)^2 (1 + M_1/M_2)^2}{8\pi a^2 N} \left[\int_0^{p_{\text{max}}/a} \sin^2\left(\frac{\theta}{2}\right) \left(\frac{p}{a}\right) d\left(\frac{p}{a}\right) \right]^{-1} \quad (2.15)$$

The integral is performed over the curve in the Figure on p. 6 appropriate to the energy E of the collision. The code also checks if $E_{\text{ionization}} (= (dE/dx)_e L)$ is $< 5\%$ of E' . If not, L is reduced until it is.

Selection of the Impact Parameter

After travelling a distance L , the projectile energy is reduced by the sum of the nuclear stopping T_{cum} and the electronic stopping, $E_{\text{ionization}}$. To determine the angular deflection and the energy transferred during the large-angle collision that occurs at the end of the free-flight path, the impact parameter must be specified. Basically, this is a method of mapping a random number between 0 and 1 onto the range 0 to ∞ .

Let $du = 2\pi p dp LN$ be the probability that the projectile finds a target atom between impact parameters p and $p + dp$ in the interval L . Divide the flight path into j increments of length $\Delta x = L/j$. Over one of these increments, the probability of *not* finding a target atom with an impact parameter between 0 and p is $1 - \pi p^2 N \Delta x = 1 - \pi p^2 NL/j$. Letting j become large, the probability v of *not* finding a target atom between 0 and p over the entire path length is:

$$v = \lim(1 - \pi p^2 NL/j)^j = \exp(-NL\pi p^2)$$

The combined probability $= v du$ of the projectile finding a target atom in (p, dp) and not between 0 and p over the flight path L is:

//

$$dw = \exp(-\pi p^2 LN) 2\pi LN p dp = e^{-n} dn$$

where $n = \pi p^2 NL$. Integrating gives $w = 1 - e^{-n}$, or $n = -\ln(1-w)$. Let w be a random number between 0 and 1; therefore $1 - w$ is also a random number between 0 and 1. Expressing n in terms of p yields the following formula for determining the impact parameter at the end of the flight path L :

$$p = \left(\frac{-\ln(1-w)}{\pi LN} \right)^{1/2} \quad (2.16)$$

where L is given by Eq (2.15). With p known, the figure on p. 6 gives θ . The lab scattering angle ϕ is obtained from Eq (2.7) and T from Eq (2.10).

Low-Energy Projectile

The free flight path given by Eq (2.15) and the impact parameter of Eq (2.16) are applied until L becomes equal to the interatomic spacing in the solid,

$$L = N^{-1/3} \quad (2.17)$$

From this point on, the maximum impact parameter is set equal to one-half of the interatomic spacing, or $p_{\max} = N^{-1/3}/2$. Since all impact parameters are equally probable:

$$p = w p_{\max} = 1/2 w N^{-1/3} \quad (2.18)$$

Where w is a random number between 0 and 1.

Equations (2.15) and (2.16) or (2.17) and (2.18) give L and p needed in steps 2 and 5 of the algorithm on page 7.

In the standard (2-dimensional) TRIM program, the energy transferred to a target atom is analyzed further to yield such results as (i) ionization by recoiling atoms in a cascade, (ii) damage energy and number of vacancies produced in a collision cascade, and (iii) damage energy and number of sub-threshold collisions in the cascade which transfer energies less than E_d , where knock-on atoms cannot permanently escape their lattice site and their energy ends up in lattice vibrations (phonons).

The recoils themselves, however, are not individually followed in this Monte Carlo program. Their energy contributions to ionization and defect production are determined by standard theory [63g] in the analytical approximation of Robinson [70j]. From this theory the defect producing energy E_v is obtained from the transferred energy T of the recoil by taking into account electronic losses

$$E_v = \frac{T}{1 + k_d g(\epsilon_d)}, \quad (4-17)$$

where the electronic losses are governed by

$$k_d = 0.1334 Z_2^{2/3} M_2^{-1/2},$$

and

$$g(\epsilon_d) = \epsilon_d + 0.40244 \epsilon_d^{3/4} + 3.4008 \epsilon_d^{1/6},$$

where

$$\epsilon_d = 0.01014 Z_2^{-7/3} T.$$

From the energy E_v the number of displacements is calculated by the well known "modified Kinchin-Pease" model (Refs. 1-3)

$$\begin{aligned} \nu &= 1, & \text{if } E_D < E_v < 2.5 E_D, \\ \nu &= \frac{0.8 E_v}{2 E_D}, & \text{if } E_v > 2.5 E_D. \end{aligned} \quad (4-18)$$

Thus, the three fractions of the recoil energy mentioned above, (i)-(iii), and the number of vacancies per depth interval are calculated and provided as standard output of the TRIM program.

1. Kinchin and R. S. Pease, Rep. Prog. Phys., vol. 18, 1 (1955).
2. P. Sigmund, Rad. Eff., vol. 1, 15 (1969).
3. M. J. Norgett, M. T. Robinson and I. M. Torrens, Nucl. Eng. Design, vol. 33, 50 (1974).

Radiation Effects

In the above section, we described the vacancy production by a modified Kinchin-Pease model applied to every recoil atom which received a transferred energy $T > E_d$, where E_d denotes the displacement energy of a lattice atom. The number of vacancies obtained by this procedure was then stored in the depth channel, where the primary knock-on atom (PKA) was created. In order to study the formation of vacancies, interstitials and replacement collisions in more detail, one has actually to follow the individual recoils through a number of collisions and generations until their energy has dropped below E_d . This way, the spatial distribution of the defects is obtained, showing often a transport of recoils (and energy) over far distances. Particularly for ion masses larger than or equal to the target atom mass, $M_1 > M_2$, the recoils may move further than the incident ion. The transport of energy could not be obtained as precisely with the semi-analytical procedures of transport theory. One of the main reasons is that the Lindhard-Nielsen-Scharff cross-section approximation $\delta\sigma(t^{1/2})$ breaks down at these low energies.

In this program, TRIMCAS, the recoils are followed through many generations (as in the sputtering case, see last section) until their energy has dropped below the displacement energy E_d . Any knock-on atom receiving more energy than E_d is considered to leave its lattice position and to create a vacancy. Thereafter a second check is performed in order to determine whether the incident particle (the ion itself or a previous recoil) is left with enough energy to move on; if its energy - after the collision - is below E_d , then it is considered to remain within the recombination volume and finally combine with the vacancy, this way annihilating the previously created vacancy and registering now as a "replacement" collision. By this process a large fraction of the vacancies may disappear again, mainly by target-target collisions at low energies. The ion-target collisions account only for a very small fraction (usually less than a percent) of all replacement collisions. If a moving particle (ion or recoil) is not ending up in a replacement collision before being slowed down to an energy less than E_d , then it will be recorded as an "interstitial" atom.