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Binary Collision Simulation of Atomic Collisions
Dynamic Composition Changes in Solids

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IPP 9/64

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Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem Max-Planck-Institut für Plasmaphysik und der Europäischen Atomgemeinschaft über die Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.

TRIDYN -

Binary Collision Simulation of Atomic Collisions

and Dynamic Composition Changes in Solids

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Program Summary

Title of program:	TRIDYN (Version 3.1)
Computer:	CRAY-XMP
Installation:	Max-Planck-Institut für Plasmaphysik
Operating system:	COS 1.16
Programming language:	FORTRAN 77
High speed storage used:	91 kwords
Number of bits in a word:	64
Peripherals used:	Line printer

Number of lines in combined program and test deck: 1661

Keywords: Atomic collisions, collision cascades, binary collision approximation, ion ranges, ion reflection, (preferential) sputtering, ion mixing, ion implantation

Nature of the physical problem:

A beam of fast ions (energy range app. 1 eV/amu to 100 keV/amu) entering a solid substance is slowed down and scattered due to electronic interaction and nuclear collisions. Along its path, an individual projectile may create fast recoil atoms which in turn may initiate collision cascades of moving target atoms. These may either leave the surface (be sputtered) or be deposited at a site different from their original one. Together with the projectiles being deposited in the substance, this results in local composition changes. In the case of large implantation fluences, these phenomena will cause collisional mixing in layered substances, changes of the surface composition due to preferential sputtering, and the establishment of a stationary range profile of the implanted ions.

Method of solution:

The paths of the individual moving particles and their collisions are modelled by means of the binary collison approximation for an amorphous substance, using a screened Coulomb potential for nuclear collisions and local or nonlocal free-electron-gas approximations for the electronic energy loss. For each nuclear collision, the impact parameter, the azimuthal deflection angle and the species of the collision partner are determined from random numbers. A proper scaling is chosen so that each incident projectile ('pseudoprojectile') represents an interval of implantation fluence. Subsequent to the termination of each pseudoprojectile and its associated collision cascades, the local partial densities of the constituents are rearranged according to their atomic volumes. In order to make advantage of vector processing, the time-consuming sections of the code have been written in vectorized form, where possible.

Typical running time:

The running time depends strongly on the problem chosen and is mainly influenced by the number of pseudoprojectiles, their energy and their atomic species. For the test example of 1 keV Ne atoms incident on Ta_2O_5, a calculation with $6 \cdot 10^4$ pseudoprojectiles corresponding to a fluence of $6 \cdot 10^{16}$ Ne/cm^2 requires 18 min on the CRAY-XMP computer.

Long Write-Up

1. Introduction

Computer simulations of atomic collisions based on the binary collision approximation have proven to be a powerful tool for about 30 years (earlier and recent reviews are found in refs. /1-4/). A number of different codes have been developed being applicable to substances of different structure, or, for example, differing in the choice of the interaction potentials. Among these programs, the TRIM code originally written by Biersack and Haggmark /5/ provides reasonably fast simulations of collisions in amorphous substances, i.e. using fixed free pathlength between subsequent nuclear collisions. Its main advantage is a fast approximative solution of the scattering integral, which derives the polar deflection angle from the randomly chosen impact parameter of the collision. In the mean time, the TRIM code became the most wide-spread one being accessible to many laboratories around the world.

Originally, TRIM had been set up for the slowing down of fast projectiles only, disregarding any target recoil atoms. (A recent version of this program is described in ref. /6/.) Later, TRIM was extended to include recoil atoms, so that simulations of sputtering could be performed with TRIM.SP /7/. A further version TRSP2C /8,9/ allowed simulations of sputtering and preferential sputtering with two-component target substances. Recently /10/, the speed of TRIM sputtering simulations could be increased considerably by means of the vectorized version TRSPV1C to be used with vector processors.

All of the TRIM simulations mentioned above are performed with a static target substance, i.e. being strictly valid only in the limit of low implantation fluences. In reality, the ion beam induces changes of the substance both due to the deposition of the projectiles and due to collisional transport, including sputtering, in polyatomic media. In order to simulate the resulting phenomena of fluence-dependent ion deposition, preferential sputtering, and atomic mixing, a 'dynamic' version of the TRIM code has been developed /11,12/ which was called TRIDYN. Its earlier, non-vectorized versions were used for preferential sputtering calculations with surprisingly good agreement with experimental findings /9,13/, proving the dominance of collisional transport in some non-metallic compounds exposed to ion-bombardment.

The present paper describes a recent vectorized version (version 3.1) of the TRIDYN program, which typically reduces the computing time by a factor of 1.5 to 2 compared to the earlier versions. It should be noted that simulations of the present type cannot be vectorized very effectively, as the calculations have to be interrupted by many checks on, e.g., particle energies and positions. Nevertheless, the above reduction is believed to be important in view of computing times of the order of one or several hours.

2. Computational Procedure

2.1 Atomic Transport

The transport of moving atoms is described in the binary collision approximation by a sequence of elastic binary collisions with the atoms of

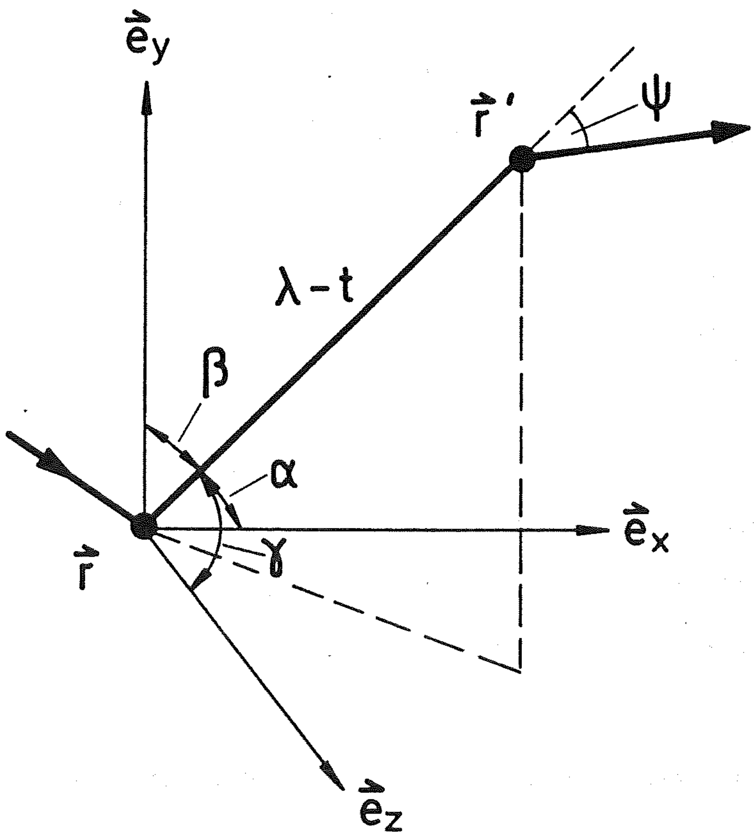

Fig. 1 Path of a moving atom with two collisions. Its direction is defined by the directional angles with respect to the unit vectors e_x, e_y, and e_z. By definition, e_x points in inward direction normal to the surface. The azimuthal scattering angle ϕ has been omitted for clarity.

the substance. In the present model for an amorphous substance, straight mean free paths are assumed between the collisions, the length λ of which is fixed for a given atomic density of the substance (see Fig. 1). Right after a collision, the state of an atom is given by its position $r = (x,y,z)$, its directional angles α, β, and γ with respect to a fixed Cartesian system, and its energy E. The locus after the subsequent collision is then given by

$$\vec{r}\,' = \vec{r} + (\lambda - t)\begin{pmatrix}\cos\alpha\\ \cos\beta\\ \cos\gamma\end{pmatrix} \tag{1}$$

where t denotes the distance of the asymptotic deflection point from the plane which is defined by the original position of the target atom (see Fig. 2). Each collision is characterized by a polar deflection angle, ψ, and an azimuthal one, ϕ. Both are determined randomly which will be described below. The new direction of the particle is then given by

$$\begin{aligned}\cos\alpha' &= \cos\psi\cos\alpha + \sin\psi\cos\phi\sin\alpha\\ \cos\beta' &= \cos\psi\cos\beta - \frac{\sin\psi}{\sin\alpha}(\cos\phi\cos\alpha\cos\beta - \sin\phi\cos\gamma)\\ \cos\gamma' &= \cos\psi\cos\gamma - \frac{\sin\psi}{\sin\alpha}(\cos\phi\cos\alpha\cos\gamma + \sin\phi\cos\beta)\end{aligned} \tag{2}$$

and its energy by

$$E' = E - T - \Delta E_l - \Delta E_{nl} \quad , \tag{3}$$

where T denotes the elastic energy transfer to the target atom, and ΔE the electronic energy losses, which may occur locally during the collisions or nonlocally along the straight paths between the collisions.

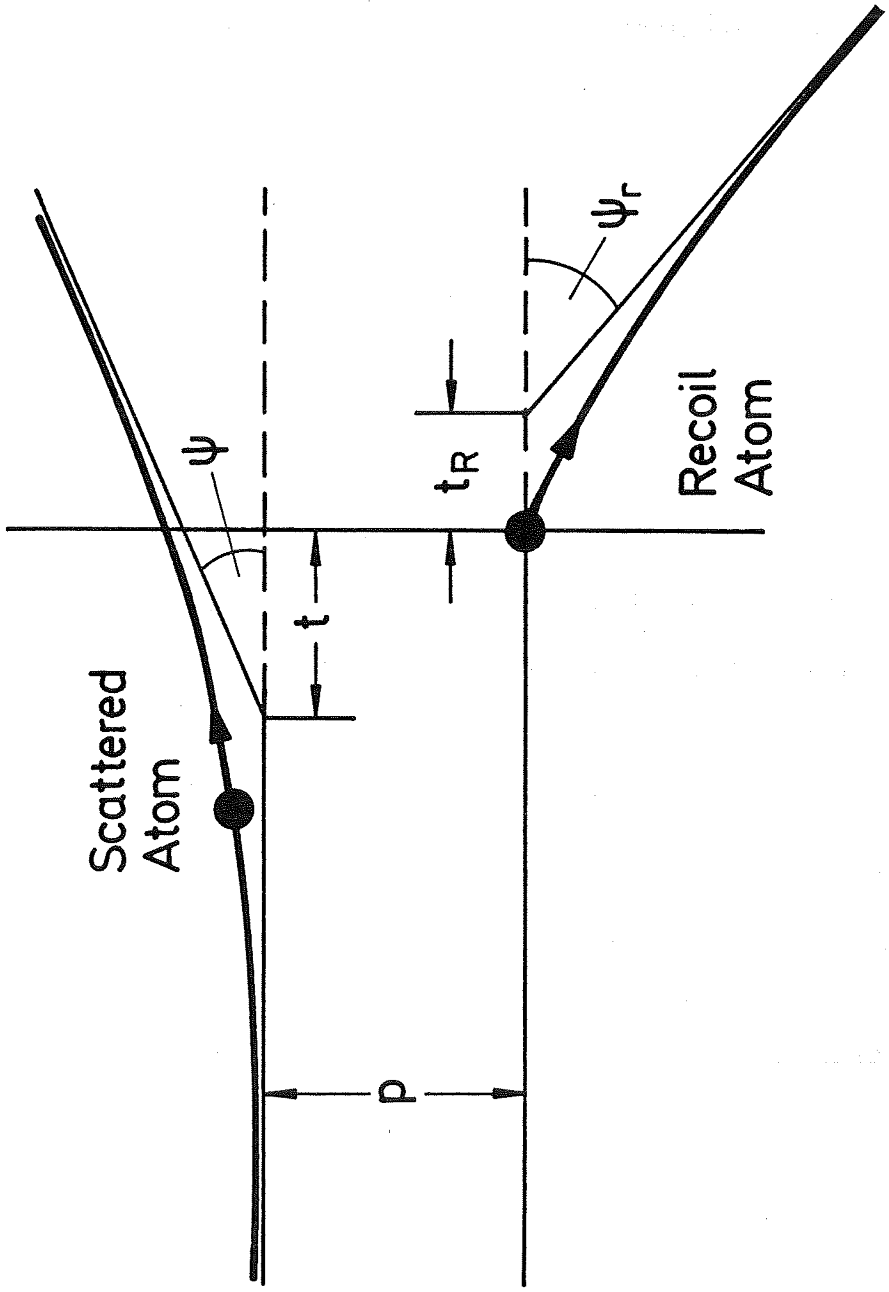

Fig. 2 Scattering geometry for an elastic two-body interaction with the target atom being initially at rest.

In eq. (1), λ is chosen from the local atomic density, n, of the substance:

$$\lambda = n^{-1/3} . \tag{4}$$

In a multicomponent substance, which is composed from N_c constituents denoted by $j = 1, \ldots, N_c$, n depends on the fractional compositions of the different atomic species, q_j:

$$n^{-1} = \sum_j q_j n_{o,j}^{-1} . \tag{5}$$

$n_{o,j}$ denote the atomic densities of the pure components; they might, however, also be chosen to fit the correct atomic density of a given compound. By definition, the fractional composition add up to unity:

$$\sum_j q_j = 1 \tag{6}$$

Whereas ΔE_{nl} depends on the local composition of the substance, ψ, T, and ΔE_l depend on the atomic mass and charge of the target atom. Therefore, its species j_b is determined before each collision randomly according to the local composition. For a given random number r_s, j_b results implicitly as

$$j_b = \min \left(j : \sum_{i=1}^{j} q_i \geq r_s\right) . \tag{7}$$

2.2 Elastic Collisions

The target atom for each atomic collision is chosen within a disc of radius p_{max} (Fig. 3). One collision takes place per atomic volume provided

$$p_{max} = (\lambda \; \pi \; n)^{-1/2} \; , \qquad (8)$$

i.e. the mean atomic volume is represented by a cylinder of length λ and radius p_{max}. The actual impact parameter p is chosen from a random number r_p according to

$$p = p_{max} \sqrt{r_p} \quad . \qquad (9)$$

The azimuthal position of the target atom within the disc is given by the azimuthal deflection angle ϕ, which is determined from its random number r_ϕ according to

$$\phi = 2\pi r_\phi \qquad (10)$$

The relation between the polar scattering angle, θ, and the impact parameter is calculated in TRIM by a fast approximation procedure /5/. According to Lindhard et al. /14/, a reduced energy is introduced by

$$\varepsilon = \frac{4\pi\varepsilon_o \; a \; m_b E}{(m_a+m_b)Z_a Z_b e^2} \qquad (11)$$

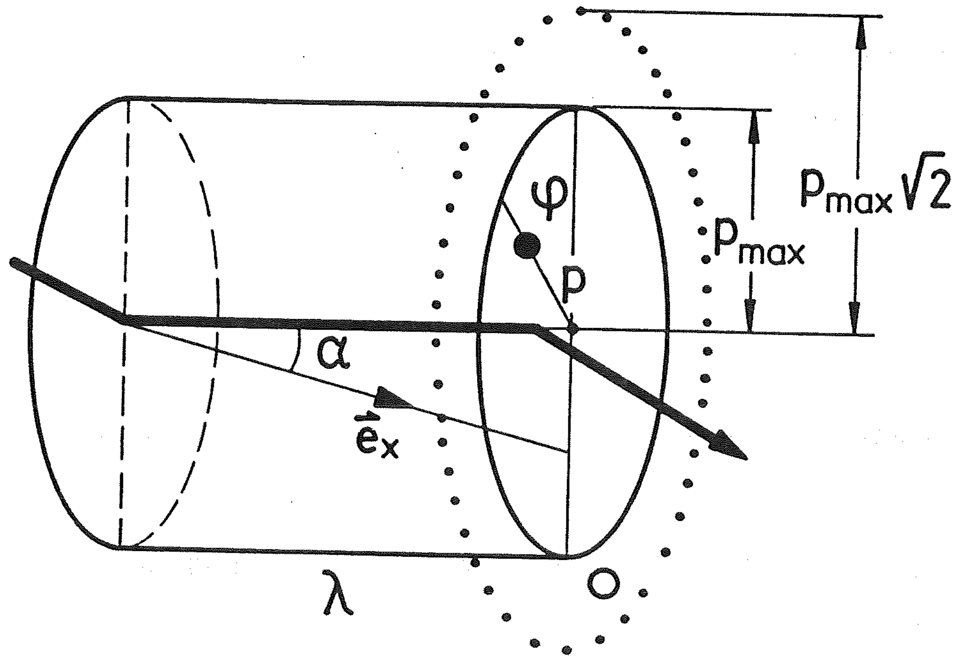

Fig. 3 Definition of the target atom position and the corresponding impact parameter p and azimuthal deflection angle, ϕ. The choice for an additional soft collision of first order is indicated by the dotted circle and the open symbol.

where (m_a, Z_a) and (m_b, Z_b) denote the atomic masses and charges of the scattered atom and target atom, respectively, and a the screening distance according to Firsov /15/

$$a = \frac{0.8853\ a_o}{(Z_a^{1/2}+Z_b^{1/2})^{2/3}} \tag{12}$$

with the radius of the first Bohr orbit, a_o = 0.529 Å. A screened Coulomb interaction potential

$$V(R) = \frac{Z_a Z_b e^2}{4\pi\varepsilon_o R}\ \phi(\frac{R}{a}) \tag{13}$$

is employed with the so-called 'Kr-C' screening function (ξ = R/a)

$$\phi(\xi) = 0.191\ e^{-0.279\xi} + 0.474\ e^{-0.637\xi} + 0.335\ e^{-1.919\xi}\ , \tag{14}$$

which represents a mean fit to individual interatomic potentials calculated for different combinations of scattering pairs by means of Hartree-Fock calculations /16/. The distance of closest approach, R_c, is calculated from

$$1 - \frac{V(R_c)}{E_c} - (\frac{p}{R_c})^2 = 0 \tag{15}$$

with the center-of-mass energy

$$E_c = \frac{m_b}{m_a+m_b}\ E\ . \tag{16}$$

In reduced form, eq. (15) can be written as ($\xi_c = R_c/a$, $b = p/a$)

$$\frac{b^2}{\xi_c} + \frac{\phi(\xi_c)}{\varepsilon} - \xi_c = 0 \ , \tag{17}$$

which is solved by Newton's method.

The deflection angle in the center-of-mass system, θ , can then be calculated according to /5/

$$\cos\frac{\theta}{2} = \frac{b + \rho + \Delta}{\xi_c + \rho} \ , \tag{18}$$

where

$$\rho = -2\,\frac{\varepsilon - \phi(\xi_c)}{\phi'(\xi_c)} \tag{19}$$

and

$$\Delta = \frac{A \cdot F}{1 + F}\,(\xi_c - b) \ , \tag{20}$$

with

$$A = 2\,(1 + \frac{C_1}{\sqrt{\varepsilon}})\varepsilon b^{(C_2+\sqrt{\varepsilon})/(C_3+\sqrt{\varepsilon})} \tag{21}$$

and

$$F = \frac{C_5+\varepsilon}{C_4+\varepsilon}\,(\sqrt{1+A^2} - A) \ . \tag{22}$$

C_1, ..., C_5 denote fitting parameters given for a specific interaction potential.

Finally, the laboratory deflection angle is determined by

$$\tan\psi = \frac{\sin\theta}{\frac{m_a}{m_b} + \cos\theta} \tag{23}$$

The offset of the deflection point (see eq. (1)) is calculated from the deflection angle in an hard-sphere approximation yielding

$$t = R_c \sin\frac{\theta}{2} \quad . \tag{24}$$

The elastic energy transfer to the target atom is given by

$$T = 4\,\frac{m_a\, m_b\, E}{(m_a+m_b)^2}\,\sin^2\frac{\theta}{2} \quad . \tag{25}$$

The above treatment allows only one collision per mean atomic distance of the substance. However, 'weak' collisions might occur with more distant atoms which might contribute to energy loss and angular deflection. The present version allows up to three additional weak collisions with impact parameters larger than p_{max}, each of them representing one additional atomic volume. In this case, eq. (9) is replaced by (k = 1,2,3):

$$p_k^{weak} = p_{max}\sqrt{k + r_p} \tag{26}$$

2.3 Inelastic Energy Loss

For low ion energies ($E \lesssim 25$ keV/amu), the electronic stopping cross section can be written according to Lindhard and Scharff /27/ as

$$S_{el} = 1.212 \frac{Z_a^{7/6} Z_b}{(Z_a^{2/3}+Z_b^{2/3})^{3/2}} \sqrt{\frac{E}{eV}} \text{ eV Å}^2 \tag{27}$$

From this, the nonlocal inelastic energy loss is calculated by

$$\Delta E_{nl} = (\lambda - t) n S_{el} , \tag{28}$$

and the local one according to Oen and Robinson /18/ by

$$\Delta E = \frac{C_6^2}{2} \frac{S_{el}}{\pi a^2} \exp(-C_6 \xi_c) \tag{29}$$

with a constant C_6 being valid for the interaction potential chosen.

2.4 Initial Conditions - Projectiles

The projectiles which initiate the collision cascades are indexed as the constituent number 1. They may start internally ($x_0 > 0$) or externally ($x_0 \leq 0$).

They might be chosen as monoenergetic (energy E_0) with a fixed angle of incidence α_0, with a two-dimensional cosine angular distribution according to

$$\cos\alpha_o = \sqrt{r_1}$$
$$\cos\beta_o = \sin\alpha_o \cos(2\pi r_2) \qquad (30)$$
$$\cos\gamma_o = \sin\alpha_o \sin(2\pi r_2) \quad ,$$

or with a random angular distribution given by

$$\cos\alpha_o = \begin{cases} 1 - r_1 \ , & x_o \leq 0 \\ 1 - 2r_1 \ , & x_o > 0 \end{cases}$$
$$\cos\beta_o = \sin\alpha_o \cos(2\pi r_2) \qquad (31)$$
$$\cos\gamma_o = \sin\alpha_o \sin(2\pi r_2)$$

from a pair of random numbers r_1, r_2. Alternatively, a Maxwellian energy-angle distribution might be chosen with an ion temperature kT_i and an additional sheath potential V_s. In this case, the squares of the velocity components read

$$v_{ox}^2 = \frac{2}{m_1} (V_s - kT_i \log r_1)$$
$$v_{oy}^2 = - \frac{2}{m_1} kT_i \cos^2(2\pi r_2) \log r_1 \qquad (32)$$
$$v_{oz}^2 = - \frac{2}{m_1} kT_i \sin^2(2\pi r_2) \log r_2 \quad ,$$

and with

$$v_o = \sqrt{v_{ox}^2 + v_{oy}^2 + v_{oz}^2} \qquad (33)$$

the directional angles and the energy result as

$$\cos\alpha_o = \frac{v_{ox}}{v_o}$$

$$\cos\beta_o = \frac{v_{oy}}{v_o} \qquad (34)$$

$$\cos\gamma_o = \frac{v_{oy}}{v_o}$$

and

$$E_o = \frac{m_1}{2} v_o^2 \quad . \qquad (35)$$

In the case of an external start ($x_0 \geq 0$), the actual start position is chosen at

$$x_s = - \frac{2}{\sqrt{\pi}} n_s^{-1/3} \quad , \qquad (36)$$

where n_s denotes the atomic density at the surface. Eqs. (4) and (8) show x_s to be twice as large as p_{max}. Furthermore, a binding energy of the projectile to the surface can be taken into account. The projectile start energy and directions are then modified according to the surface binding energy of the projectile, $E_{s,1}$:

$$E_0' = E_0 + E_{s,1} \qquad (37)$$

and

$$\cos\alpha_o' = \left(\frac{E_o \cos^2\alpha_o + E_{s,1}}{E_o + E_{s,1}}\right)^{1/2}$$

$$\cos\beta_o' = \cos\beta_o \frac{\sin\alpha_o'}{\sin\alpha_o} \qquad (38)$$

$$\cos\gamma_o' = \cos\gamma_o \frac{\sin\alpha_o'}{\sin\alpha_o} \quad .$$

Any projectile starting externally is assumed to enter an 'atomically rough' surface. Accordingly, its first position of collision is determined from a random number r by

$$x_1 = x_c + \lambda r \cos\alpha_o'$$

$$y_1 = \lambda\, r \cos\beta_o' \qquad (39)$$

$$z_1 = \lambda\, r \cos\gamma_o'$$

2.5 Recoil Generation

By any hard collision of a projectile or recoil atom with a target atom of species j_b, a new recoil may be generated provided the elastic energy transfer T is larger than the bulk binding energy, E_{b,j_b}. Its initial energy is then

$$E_{bo} = T - E_{b,jb}. \qquad (40)$$

The start position is given by the locus of the collision, as the asymptotic offset t_R (see Fig. 2) vanishes in case of the hard sphere approximation. Its directional angles with respect to the original direction of the scattered particle are given by

$$\tan \psi_r = \frac{\sin\theta}{1-\cos\theta} \tag{41}$$

and

$$\phi_r = \pi - \phi \quad . \tag{42}$$

2.6 Boundary Conditions

Any particle of species j moving in front of the surface between x = 0 and $x = x_s$, is still allowed to interact with the substance in order to include weak external deflections. However, an emerging particle exceeding x_s will be subject to boundary conditions imposed by the model of a planar surface threshold. Provided the normal fraction of its energy, $E\cos^2\alpha$, is smaller than the surface binding energy, $E_{s,j}$, the atom will reenter the surface with the new direction

$$\cos\alpha' = -\cos\alpha \quad . \tag{43}$$

Alternatively, the atom is regarded as reflected (in case of an incident projectile) or sputtered (in case of a recoil atom). Then, the emerging energy is modified according to

$$E' = E - E_{s,j} \quad . \tag{44}$$

If statistics on the emerging directions are desired, the final directions may be obtained in a way similar to eq. (38). This is not included in the present version of TRIDYN. It does neither include a corresponding treatment of transmitted particles in case of thin films.

2.7 Particle Termination

The history of a moving particle of species j is terminated when it has been slowed down to an energy below a predefined cutoff energy, $E_{f,j}$. In order to obtain reflection and sputtering yields correctly, $E_{f,i}$ ($i = 1, \ldots, N_c$) have to be chosen equal to or smaller than the surface binding energies, $E_{s,i}$.
The final position of an incident projectile is taken equal to its last recorded depth. However, in case of a recoil atom, one may decide to treat it as 'free' or 'bound'. In the latter case, it will be put back to its depth of origin, provided its starting energy had been lower than its displacement threshold, $E_{d,j}$. In this way, the program may treat energy transport without mass transport.

2.8 Radiation Damage

The present program calculates a mean number of Frenkel pairs for each primary collision between a projectile and a target atom of type j according to the modified Kinchin-Pease model /19/

$$N_F(T) = \begin{cases} 0 & T \leq \overline{E_d} \\ 1 & E_d \leq T \leq 2.5\,\overline{E_d} \\ \dfrac{0.8\,\nu(T)}{2\overline{E}_d} & T \geq 2.5\,\overline{E_d} \end{cases} \qquad (45)$$

where $\nu(T) \simeq 0.9\ T$ denotes the fraction of the primary recoil energy which is not dissipated into electronic losses. The mean displacement threshold energy is calculated by

$$E_d^{-1} = \sum_i q_i\, E_{d,i}^{-1} \quad . \tag{46}$$

In addition, the Frenkel pairs of each component generated both by primary events and in the collision cascades are recorded, being represented by the corresponding number of recoil atoms set in motion with an energy above the displacement threshold.

2.9 Composition of the Substance

Many of the equations in sects. 2.1 to 2.8 depend on the local composition of the substance. An inhomogeneous substance can be treated by subdividing the substance into N slabs of initially constant thickness, Δx_0. As it will be seen below, the depth intervals might be changed to nonequidistant ones during the calculation. However, outputs of dynamic composition profiles are calculated for equidistant intervals by interpolation.

2.10 Dynamic Relaxation

The principle of the dynamic relaxation of the target substance is depicted in Fig. 4. Each projectile or moving particle in the computer simulation ('pseudoparticle') represents an interval of fluence. If an implantation procedure with a total fluence Φ_{tot} is simulated by a computer simulation

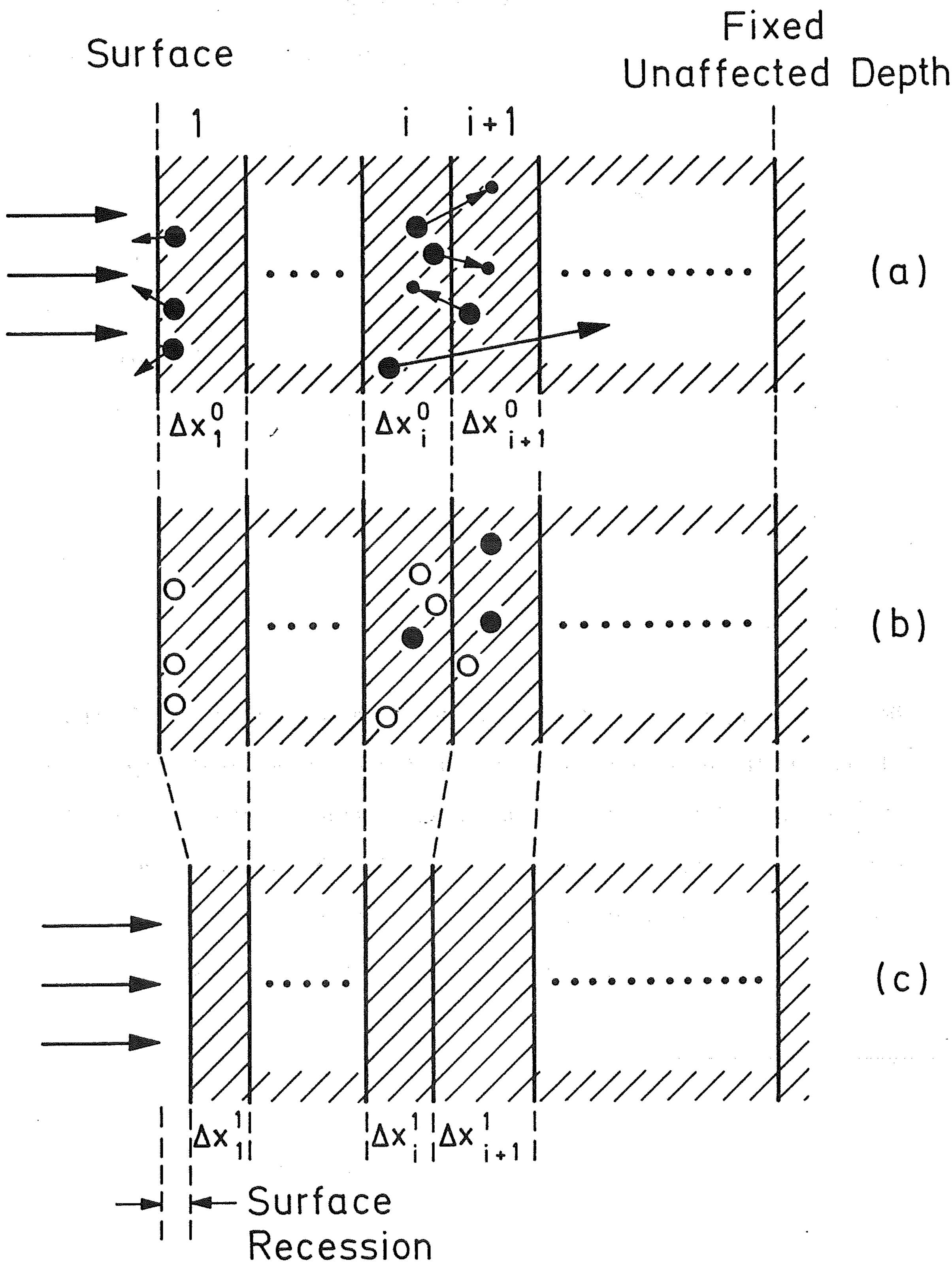

Fig. 4 Schematic representation of collisional transport and dynamic relaxation: Relocations and sputtering caused by bombardment (a) produce vacancies and additional atoms (b), which are allowed to relax (c).

employing N_H incident pseudoprojectile histories, each pseudoparticle represents a differential fluence of

$$\Delta\Phi = \frac{\Phi_{tot}}{N_H} \tag{47}$$

TRIDYN performs the following procedure subsequent to the termination of each pseudoprojectile history. The collision cascades, and the slowing down of the projectile may cause the removal or the deposition of pseudoparticles in different depth layers due to sputtering, atomic relocation, and implantation. Denoting the change of the number of pseudoparticles of type j in each layer i (i = 1, ..., N) by ΔN_{ij}, the new areal densities of real atoms in that layer are given by

$$A_{ij} = q_j n_i \Delta x_i + \Delta N_{ij} \Delta\Phi \quad . \tag{48}$$

For j = 1 (the incident projectile species), a maximum allowed atomic fraction q_1^{max} can be defined in order to simulate local saturation phenomena. The maximum areal density of constituent 1 is then

$$A_{i1}^{max} = \frac{q_1^{max}}{1-q_1^{max}} \sum_{j=2}^{N_c} A_{ij} \quad . \tag{49}$$

If $A_{i1} > A_{i1}^{max}$, an incremental flux of reemitted projectiles is defined by

$$\Delta A_{i1}^{reem} = A_{i1} - A_{i1}^{max} \quad . \tag{50}$$

and eq. (48) (for j = 1) is replaced by

$$A_{i1} = A_{i1}^{max} \quad . \tag{51}$$

From the above procedure, there arise local excess densities or depletions. These are allowed to relax by adjustment of the interval thicknesses:

$$\Delta x_i = \sum_{j=1}^{N_c} A_{ij} \, n_{o,j}^{-1} \tag{52}$$

The incremental surface recession per pseudoprojectile results naturally as the difference of the integrated slab thicknesses,

$$d_{tot} = \sum_{i=1}^{N} \Delta x_i \quad , \tag{53}$$

before and after that pseudoprojectile passage.

The thickness of the individual slabs is always held between $0.5 \cdot \Delta x_0$ and $1.5 \cdot \Delta x_0$. A too narrow interval is combined with its next neighbour; a new interval N is then fetched into the calculation with the atomic fractions of the last interval at the beginning of the simulation. A too large interval is split into two smaller ones, and the last interval is discarded.

Finally, the new atomic fractions are calculated according to

$$q_{ij} = \frac{A_{ij}}{\sum_k A_{ik}} \quad , \tag{54}$$

and the new local atomic densities according to eq. (5).

The statistical quality of the dynamic relaxation procedure depends on the choice of the number of pseudoprojectiles for a given total fluence of projectiles. As a figure of experience, the maximum relative change of the areal density in any layer

$$\left(\frac{\Delta A}{A}\right)_{max} = \max\left(\frac{\Delta\Phi \sum_{j=1}^{N_c} \Delta N_{ij}}{n_i \Delta x_i} \quad , \; i=1,\ldots,N\right) \tag{55}$$

should not exceed 5% during the complete simulation.

3. Program Description

3.1 Numerical Procedure

The TRIDYN program consists mainly of one module only in order to save computer time which otherwise would be needed for subprogram calls. Where useful and possible, the equations have been written in vectorized form. As the dynamic relaxation procedure is performed subsequent to each pseudo-projectile history, parallel computing is not possible for the incident projectiles.

The main blocks of the program are shown in Fig. 5. Initially, constants are preset from the input data, and the projectile history loop is entered to be run N_H times. Details of the projectile history and the projectile loops are given in Figs. 6 and 7, respectively. The projectile loop is entered with the locus of the first collision. After determining the actual depth interval and the corresponding local quantities, the weak collision loop is entered which finally defines new directions after each of the simultaneous collisions. (Actually, the last passage of the weak collision loop represents the hard collision.) A primary recoil may be generated and stored for each hard collision. The projectile loop is left after termination of the projectiles' history with the primary recoil atoms having been generated stored in list 1.

The collision cascade loop is essentially of the same structure as the projectile loop. Its vectorized equations, however, allow a simultaneous treatment of recoil atoms over large fractions of the loop. The loop is

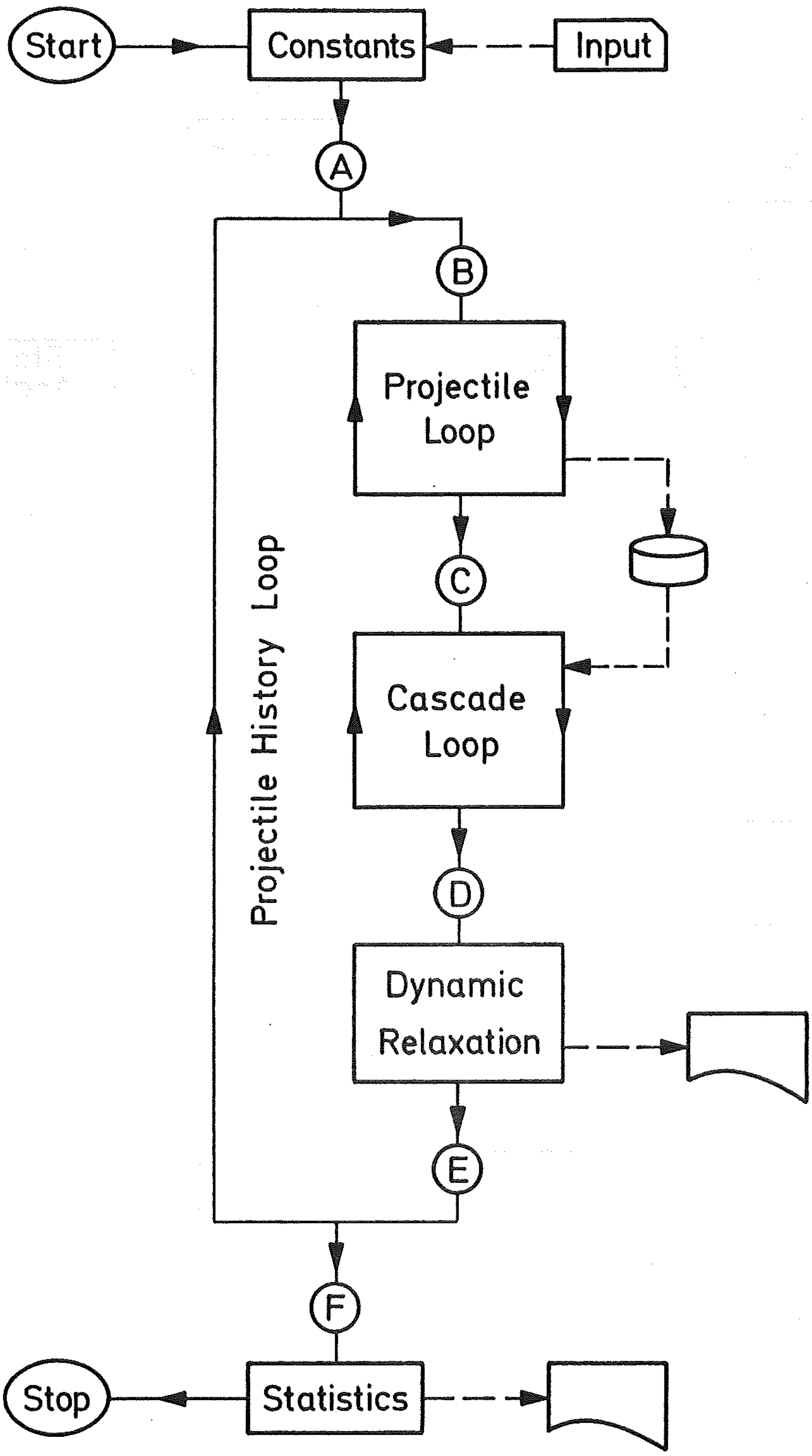

Fig. 5 Block flow chart of TRIDYN. (A) to (F) denote the connection points of the different units.

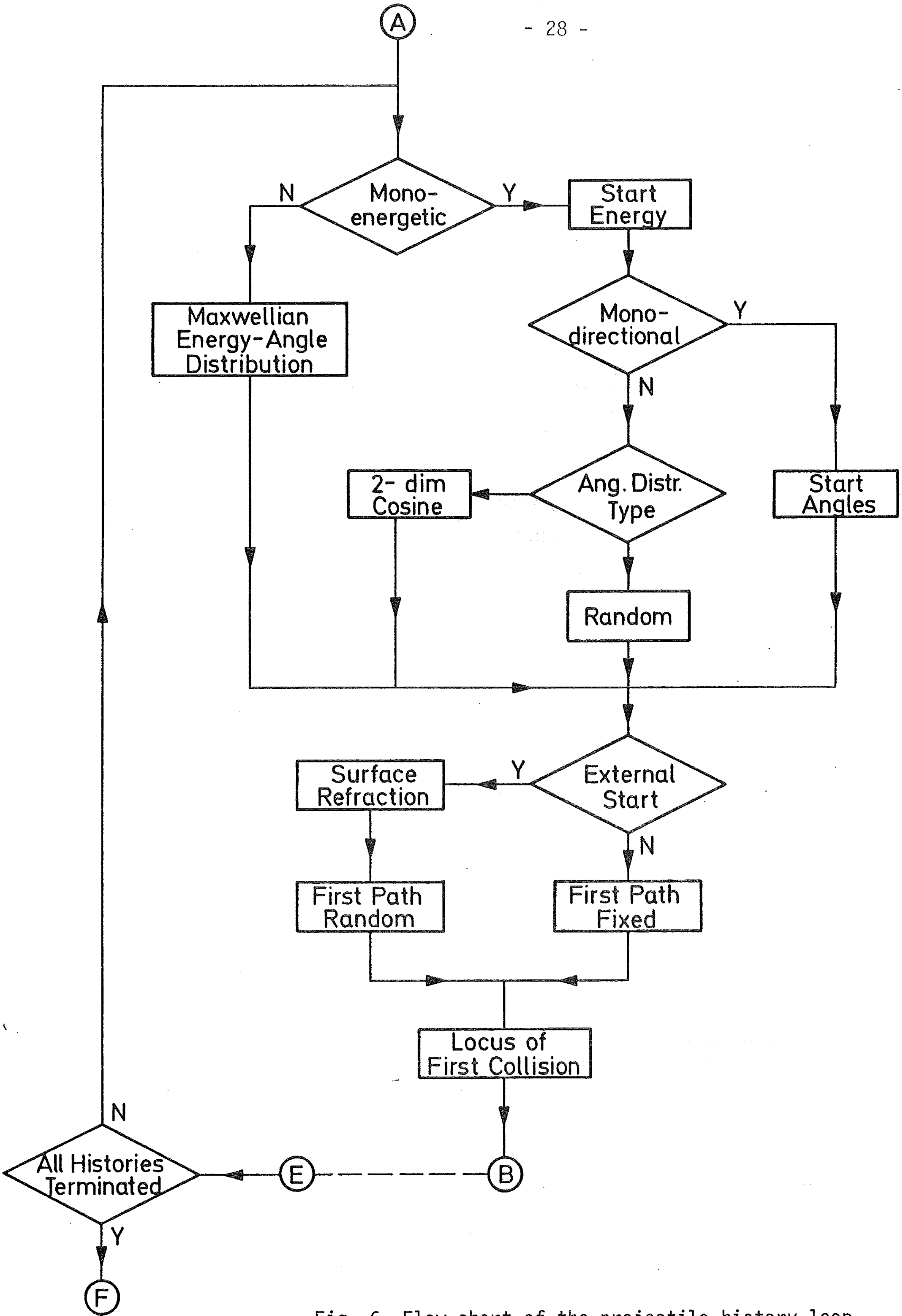

Fig. 6 Flow chart of the projectile history loop.

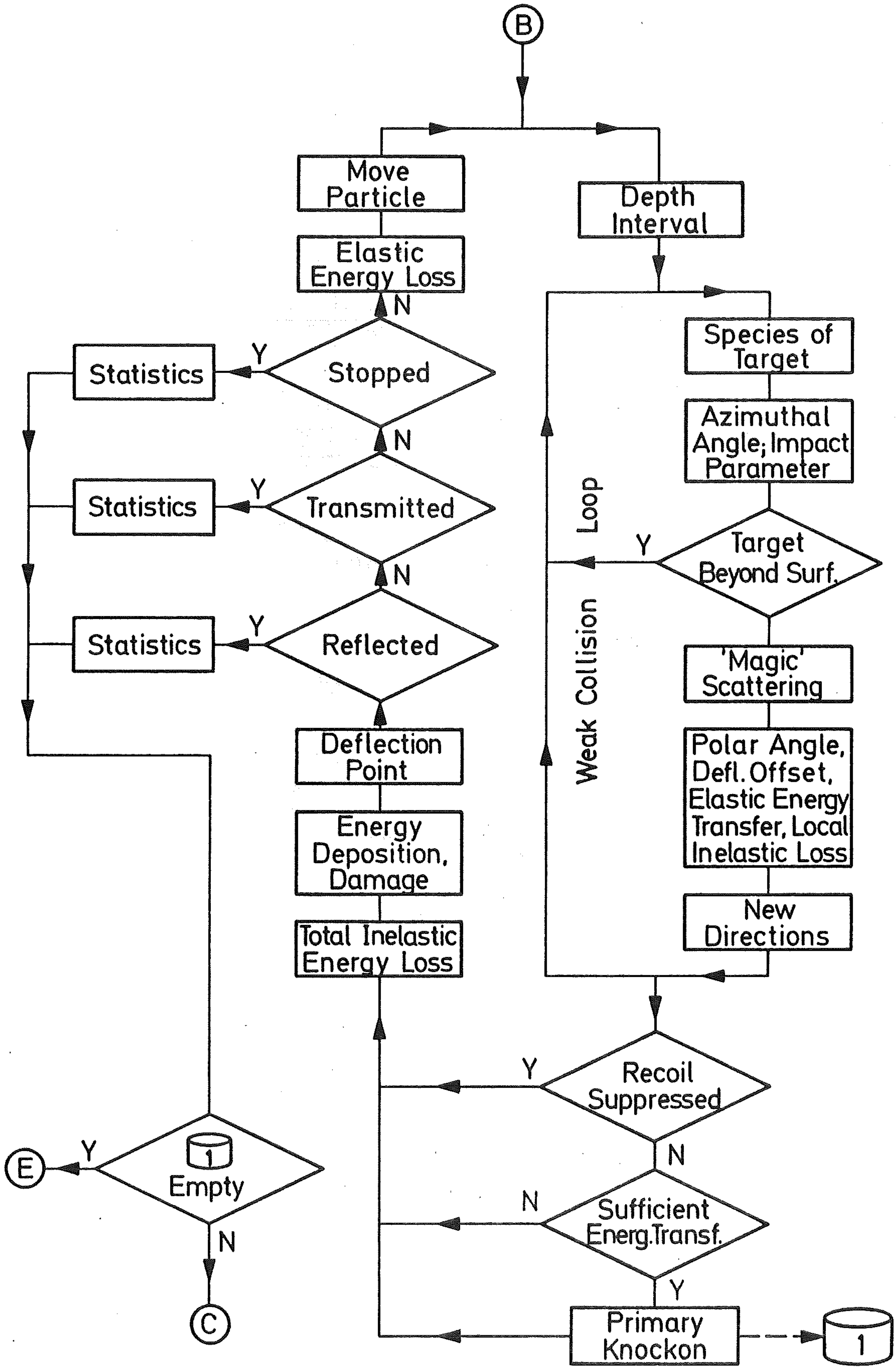

Fig. 7 Flow chart of the projectile loop. Primary knockon atoms generated during the projectile history are stored in list 1.

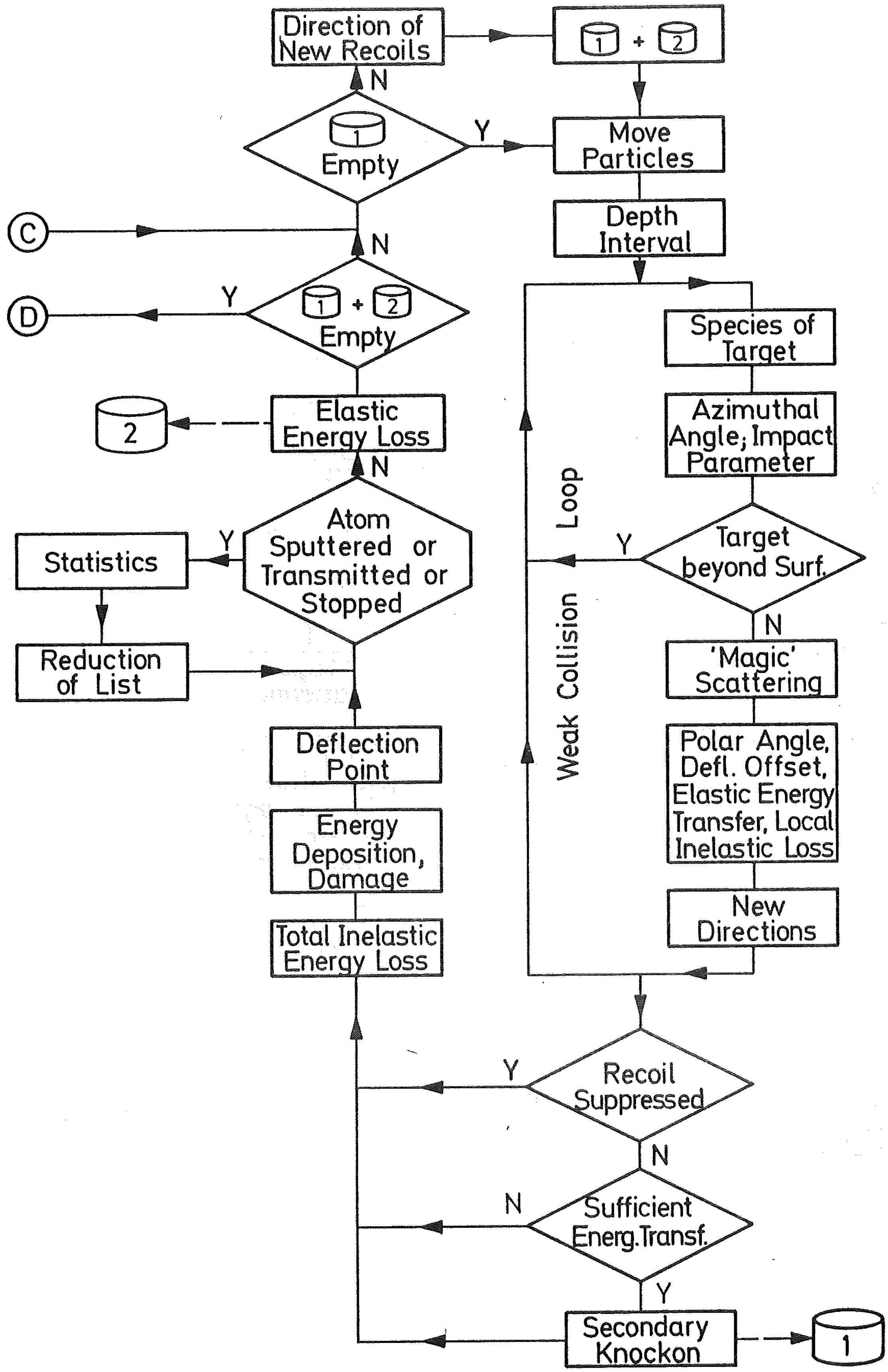

Fig. 8 Flow chart of the vectorized collision cascade loop. The loop starts with the list 1 primary recoils generated in the projectile loop.

started with the primary recoils from list 1, being transferred to list 2. Secondary recoils generated are again stored in list 1. Upon termination of a recoil history, list 2 is correspondingly reduced. It is combined with the new recoils from list 1 for the subsequent passage of the loop. The loop is terminated when both list 1 and list 2 are empty.

The dynamic relaxation section (Fig. 9) determines the new depth intervals and the correspondig atomic compositions and densities according to sect. 2.10. At its end, the pseudoprojectile deposition profiles are readjusted with respect to the surface recession. After a predefined number of pseudoprojectile passages, this section also provides the output of the dynamic composition profiles and corresponding integral quantities like sputtering and reemission yields, surface recession, surface concentrations and total areal densities.

After having terminated the desired number of pseudoprojectile histories, the program enters a section which was taken over from nondynamic TRIM versions. Here, deposition functions of the pseudoprojectiles together with some of their moments are calculated, together with statistics on sputtered and reflected particles. The corresponding output is performed. Finally, output data sets are calculated for projectile range and energy deposition profiles, and damage profiles, now being converted to atomic units.

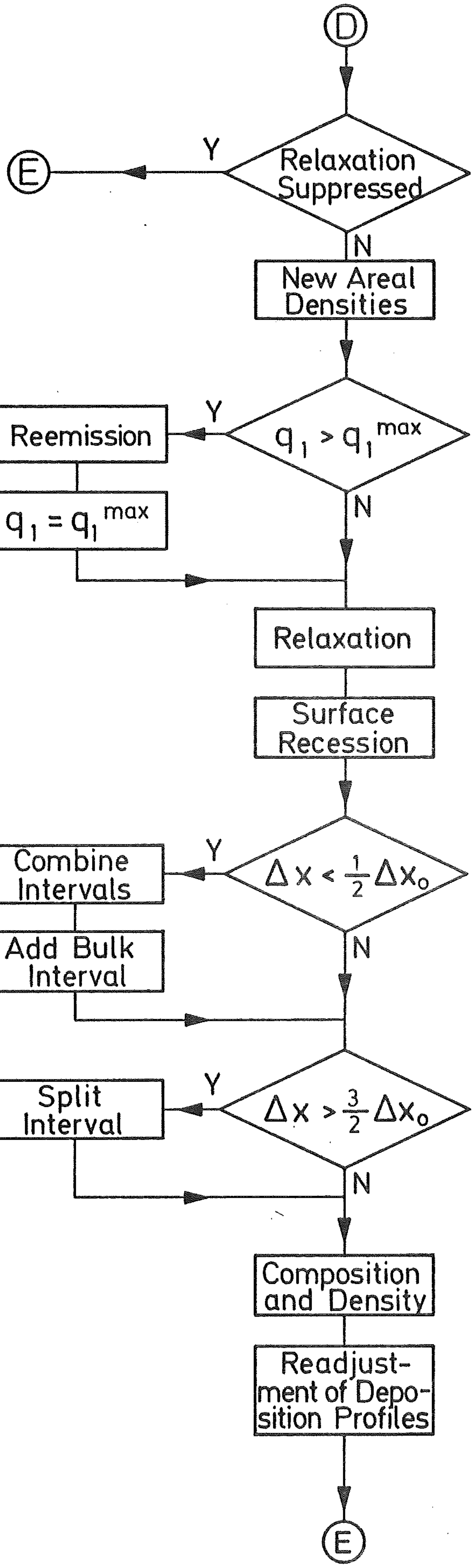

Fig. 9 Flow chart of the dynamic relaxation section.

3.2 Important and Frequently Occuring Variables

In the following, variables are listed which denote the important physical and computational variables. Some of them occur both as scalars in the projectile loop and as vectors in the recoil loop; the latter are denoted by an index IV and may occur both in list 1 and in list 2 as described above (index IL). Depth-dependent arrays are denoted by the index ID, the different constituents of the substance by IC. Note that the length unit is 10^{-10} m, and the energy unit eV.

General Constants

NH	- total number of projectile histories
FLC	- total projectile fluence
TT	- thickness of target substance
TTDYN	- max. depth of calculation
NQX	- number of depth intervals
DQX	- initial depth spacing
NCP	- number of different constituents

Properties of Constituents

ZZ(IC)	- atomic number
M(IC)	- atomic mass
SBE(IC)	- surface binding energy
BE(IC)	- bulk binding energy
ED(IC)	- displacement threshold energy
EF(IC)	- cutoff energy
CK(IC)	- correction factor for projectile electronic stopping
DNSO(IC)	- inverse of atomic volume

QU1MX	- maximum atomic fraction of component 1 (projectile)

Depth-Dependent Arrays

XNO(ID)	- depth grid
DNS(ID)	- total atomic density
QUX(ID,IC)	- atomic fraction
DEL(ID,IC)	- change of number of pseudoparticles per layer; also areal density

Collisional Constants

MU(IC_a,IC_b)	- mass ratio
EC(IC_a,IC_b)	- elastic energy transfer factor
A(IC_a,IC_b)	- screening distance
F(IC_a,IC_b)	- energy scaling factor
KL(IC_a,IC_b)	- nonlocal electronic stopping factor
KOR(IC_a,IC_b)	- local electronic stopping factor

Collisional Variables

LM,LMV(IV,IL)	- free path length
PMAX,PMAXV(IV)	- maximum impact parameter
P,PR(IV)	- impact parameter
B,BR(IV)	- reduced impact parameter
EPS,EPSR(IV)	- reduced energy
R,RRV(IV)	- reduced distance of closest approach
PHI,PHIR(IV)	- azimuthal deflection angle
C2,C2R(IV)	- $\cos^2\frac{\theta}{2}$, θ polar deflection angle (center-of-mass system)
S2,S2R(IV)	- $\sin^2\frac{\theta}{2}$

PSI,PSIR(IV,IL)	- polar deflection angle (laboratory system)
DEN,T(IV)	- elastic energy transfer
DENS,TS(IV)	- weak and hard collision sum of elastic energy transfers
TAU,TAUR(IV)	- deflection point offset
DEEOR,DEEROR	- local inelastic energy transfer
DEES,DEERS(IV)	- sum of local inelastic energy transfers

Moving Atom State and Flags

E,ER(IV,IL)	- energy
COSX,CSXR(IV) COSY,CSYR(IV) COSZ,CSZR(IV)	- directional cosines
SINE,SNXR(IV)	- directional sine, x-direction
X,XR(IV,IL) Y,YR(IV,IL) Z,ZR(IV,IL)	- position (x normal to surface)
IXST(IV,IL)	- depth interval of origin
EORC(IV,IL)	- recoil start energy
INOUT(IV,IL)	- flag for in-outgoing projectile at primary recoil generation
KO(IV,IL)	- primary or secondary knockon flag
LABEL(IV,IL)	- atomic species
L(IV,IL)	- depth of origin

Deposition Profiles and Statistics

IRP(ID)	- range of pseudoprojectiles
IPL(ID)	- pathlength of pseudoprojectiles
NCLR(ID)	- nuclear energy deposition of pseudoprojectiles
PHON(ID)	- nuclear energy deposition of pseudoprojectiles below displacement threshold
DMGN(ID)	- nuclear energy deposition of pseudoprojectiles above displacement threshold
ION(ID)	- electronic energy deposition of pseudoprojectiles
FPKP(ID)	- number of Frenkel pairs generated by pseudoprojectiles (Kinchin-Pease model)
BBR(ID,IC)	- number of Frenkel pairs generated in all collisions (including cascades)
BBRTOT(IC)	- total number of Frenkel pairs of each component
IB	- total number of reflected pseudoprojectiles
EB	- total energy of reflected pseudoprojectiles
IBSP(IC)	- total number of sputtered pseudoatoms
EBSP(IC)	- total energy of sputtered pseudoatoms
IPREC	- total number of pseudoprojectiles being removed from range profile due to surface recession

3.3 Subprograms

The following subroutines are employed (those denoted by '(L)' are CRAY library routines):

CVMGT(A1,A2,LOG) - Function assigning A1 if LOG = .TRUE. or A2 if LOG = .FALSE. (L)

DIRCOS(COSX,COSY,COSZ,SINE,PSI,PHI) - Subroutine determining new directions from old ones and deflection angles

DIRCOSV(COSX,COSY,COSZ,SINE,PSI,PHI,N) - same as DIRCOS but for a vector of length N

ILLZ(N,TEST,1) - Function returning the number of leading .FALSE. components of a logical array TEST of length N (L)

ILSUM(N,TEST,1) - Function returning the total number of .TRUE. components of a logical array TEST of length N (L)

ISMAX(N,A,1) - Function returning the index of the maximum component of an array A of length N (L)

ISCHRFGE(N,A(1),1,X) - Function returning the first index where $A(I) \geq X$ for an array A of length N (L)

MXVELO(E,COSX,COSY,COSZ,SINE) - Subroutine for random generation of energy and directions from a Maxwellian distribution

RANF( ) - Random number generator (L)

RANSET(IRAND) - Random number initialization (L)

TRUNC(A,F,N,M) - Truncation of an array A of length N for trailing zeroes and multiplying it by the elements of an array F of length N. The new dimension is M.

4. Input and Output

Channel 5 is used for the program input data. A detailed explanation of the input data and their formats is given in the program listing.

A lineprinter output is assigned to channel 6. It contains a reproduction of the input data, followed by a list of collisional constants. In the subsequent lines, the following quantities are given:

SIMREC - the maximum number of recoils treated simultaneously (maximum length of list 2)

TOTREC - the total number of recoils treated

MAXCHA - the maximum relative change of areal density in any interval of depth (eq. (55))

Furthermore, the final surface recession and the areal density of reemitted projectiles are printed. The remaining printer output concerns pseude-particle statistics, with numbers not having been converted to areal densities or local concentrations. It lists the total numbers of reflected (backscattered) pseudoprojectiles, transmitted ones and those which have been removed from the range profile due to surface recession. Sputtered pseudoparticles are classified with respect to their species and their history of origin (generated as primary or secondary knockon atoms by in- or outgoing projectiles). For the pseudoprojectiles, four moments of their range profile and two moments of their pathlength distribution are given, as well as integral energy transfer and damage quantities. These data are not corrected for surface recession. Finally, the corrected range, pathlength and energy deposition profiles of pseudoprojectiles are listed.

An additional output file on channel 17 contains the projectile deposition profiles and damage profiles in atomic units, normalized to the predefined total fluence. The output format is described in the program listing.

The result of the dynamic composition simulation is given on channel 7. At the beginning of the run and after termination of IDOUT pseudoprojectiles each, a four-record listing of integral quantities is provided. In addition, the composition and local density profiles are listed after termination of IQOUT pseudoprojectiles each. A detailed explanation is given in the program listing. The first two lines of the file contain a headline and the quantities NH, IDOUT, IQOUT, NCP, NQX, and the program name.

5. Test Run

As the test problem, the bombardment of Ta_2O_5 with 1 keV Ne ions at a fluence of $6 \cdot 10^{16}$ Ne/cm^2 has been chosen. The maximum Ne atomic fraction is arbitrarily set to 0.2. The runtime is about 18 min on the CRAY-XMP.

Fig. 10 shows the evolution of the composition profiles with the buildup of the Ne profile to saturation and the change of Ta profile due to preferential sputtering and collisional relocation. Correspondingly, the host surface composition and the amount of retained projectiles are displayed in Fig. 11 as functions of the implantation fluence. Finally, the partial sputtering yields of all components are given in Fig. 12.

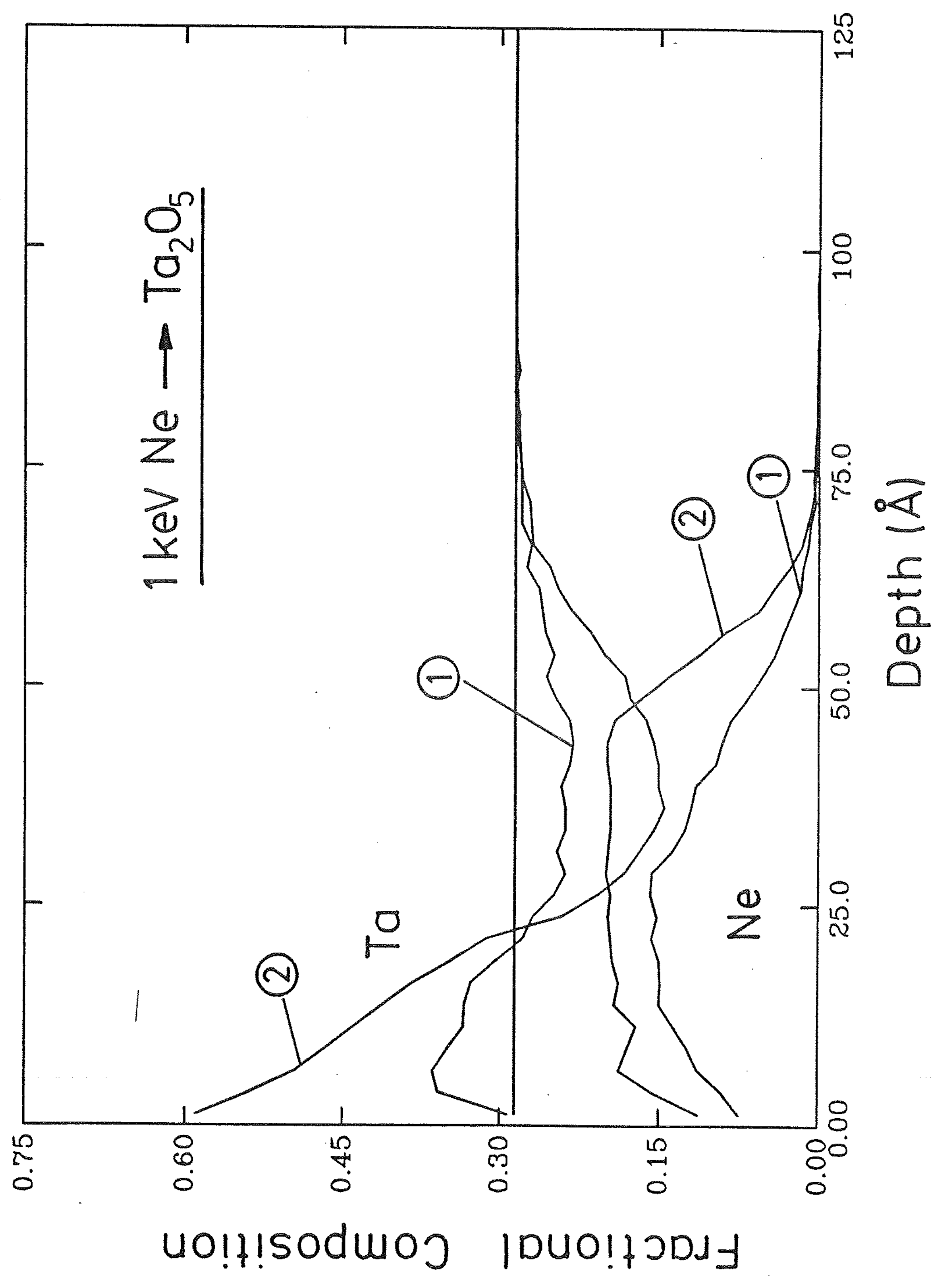

Fig.10 Initial, intermediate and stationary composition profile from the test run. The fluences are $6 \cdot 10^{15}$ Ne/cm^2 (denoted by ①), , and $6 \cdot 10^{16}$ Ne/cm^2 (②).

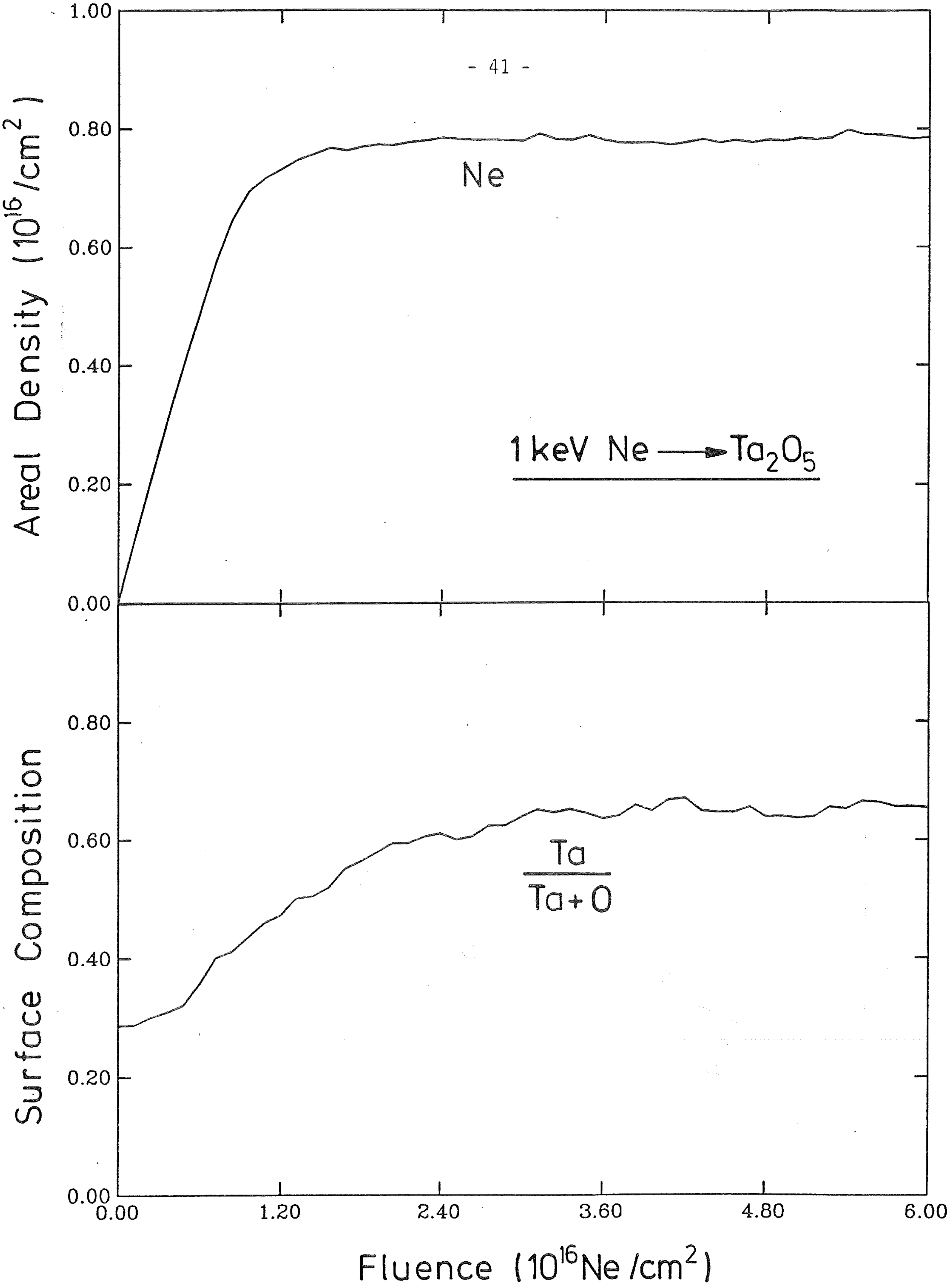

Fig.11 Surface composition of the host elements (integrated over 5 Å) and retained amount of implanted projectiles as function of fluence from the test run.

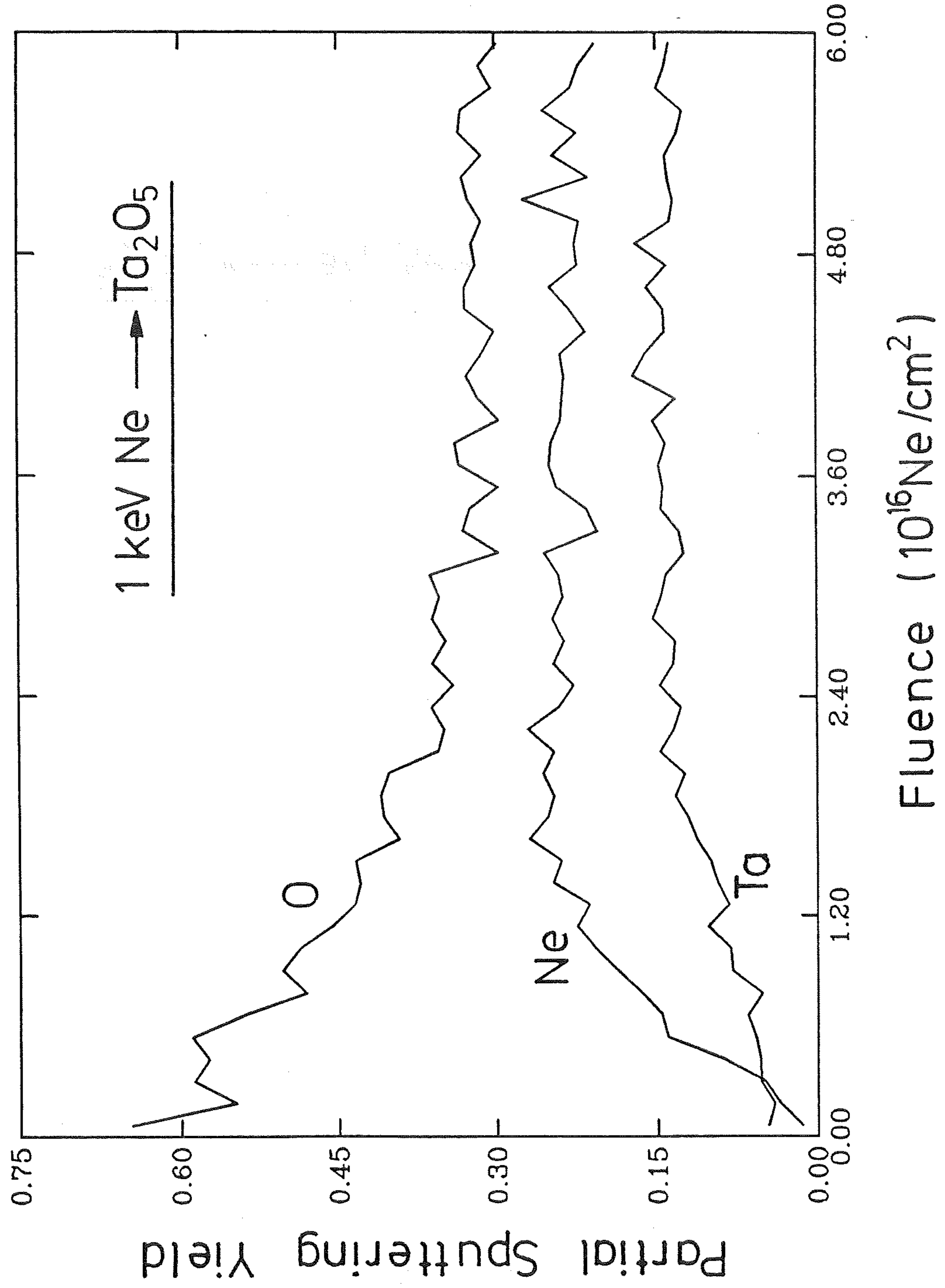

Fig.12 Partial sputtering yields as function of fluence from the test run.

6. Limitations

TRIDYN has proven to be a powerful tool for the study of collisional effects occuring during ion bombardment of solids. Its application is, however, limited by several constraints:
For very low energies ($\lesssim$ 1 eV/amu), the validity of the binary collision approximation becomes extremely questionable. Therefore, the final thermalization of collision cascades cannot be treated. This would require molecular dynamics computer simulations; at present there is, however, no chance to calculate dynamic composition changes by molecular dynamics models due to time limitations.

For high energies (> 1 keV/amu), TRIDYN may be used in principle, but with often excessively long computing times. For this reason, the nonlocal electronic stopping power employed in the program is only valid for sufficiently low energies ($\lesssim$ 25 keV/amu), which should not be exceeded when using the program.

Finally it should again be stressed that dynamic composition studies by TRIDYN are only valid for systems which are dominated by collisional effects. Any chemical phenomena, especially thermal or ion-induced diffusion, segregation or precipitation are not included in a computer simulation of the present type.

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Appendix 1

Listing of the Program

```
C
C
C
C     PROGRAM TRIDYN      VERSION 3.1
C
C     DYNAMIC COMPOSITION TRIM PROGRAM
C
C     W.MOELLER   IPP/OP   JAN.1988   CRAY-XMP
C
C     VECTOR COMPUTER VERSION
C
C     BASED ON 1-COMPONENT SPUTTER-TRIM TRSPTC1 (J.P.BIERSACK AND
C     W.ECKSTEIN), VECTORIZED SPUTTER-TRIM TRSPV1CT (W.ECKSTEIN),
C     AND 5-COMPONENT DYNAMIC COMPOSITION TRIM PROGRAM TRIDYN,
C     VERSION 2.3 (W.MOELLER)
C
C
C
C
C     INPUT DATA (CHANNEL 5)
C
C     TITLE RECORD (FORMAT 16A4):
C
C     64-CHARACTER TITLE OF CALCULATION
C
C     1.RECORD (FORMAT I10,11I5):
C
C     NH         NUMBER OF PROJECTILE HISTORIES
C     IDOUT>0    DATA OUTPUT AFTER EACH IDOUT'TH HISTORY
C          <=0    OUTPUT SUPPRESSED
C     IQOUT      ADDITIONAL PROFILE OUTPUT AFTER EACH IQOUT'TH HISTORY
C     NCP        NUMBER OF TARGET COMPONENTS (INCLUDING PROJECTILE)
C     IDREL>0    SUPPRESSION OF DYNAMIC RELAXATION
C          <0    SUPPRESSION OF DYNAMIC RELAXATION AND CASCADES
C     IQ0<0      INITIAL COMPOSITION VARIABLE ACCORDING TO VECTOR INPUT
C        =0      INITIAL COMPOSITION HOMOGENEOUS
C        >0      INITIAL COMPOSITION ACCORDING TO LAYER INPUT
C     IRC0<0     SUBTHRESHOLD RECOIL ATOMS FREE
C         >=0    SUBTHRESHOLD RECOIL ATOMS BOUND
C     IRAND      INITIAL RANDOM NUMBER
C     JSP1,JSP2 SUPPRESSION OF RECOILS OF TYPE JSP1,...,JSP2
C       JSP1=0  ALL RECOILS TRACED
C     JFRP       FRENKEL PAIR GENERATION FOR COMPONENTS JFRP,...,NCP
C                (DEFAULT: NCP)
C     JNRM       NORMALIZATION OF PUNCH1 OUTPUT TO PARTIAL DENSITY OF
C                COMPONENTS JNRM,...,NCP (DEFAULT: NCP)
C
C     2.RECORD (FORMAT E10.3,3F10.2,4I5,F10.2):
```

```
C
C     FLC        IMPLANTED FLUENCE (1E16/CM2) FOR COMPLETE RUN
C     E0         PROJECTILE ENERGY (EV)
C       <0:      MAXWELLIAN ENERGY-ANGLE DISTRIBUTION WITH KT=-E0
C                (ALPHA IS IGNORED IN THIS CASE)
C     X0         PROJECTILE START DEPTH (A)
C     ALPHA      ANGLE OF INCIDENCE (DEG) WITH RESPECT TO NORMAL
C        = -1:   RANDOM ANGLE DISTRIBUTION
C        = -2:   2-DIMENSIONAL COSINE DISTRIBUTION
C     INEL =1    INELASTIC PROJECTILE-TARGET INTERACTION NONLOCAL
C           2                                            LOCAL
C           3                                            EQUIPART.
C     INELR      INELASTIC TARGET-TARGET INTERACTION (SEE INEL)
C     IWC        MAX. ORDER OF WEAK PROJECTILE-TARGET COLLISIONS
C     IWCR       MAX. ORDER OF WEAK TARGET-TARGET COLLISIONS
C     SHTH       SHEATH POTENTIAL (EV) IN CASE OF MAXWELLIAN
C                ENERGY DISTRIBUTION
C
C     3.RECORD (FORMAT 2E10.3,I5,E10.3,3I5):
C
C     TT         TARGET THICKNESS (A)
C     TTDYN      DEPTH RANGE (A) FOR DYNAMIC RELAXATION
C     NQX        NR. OF DEPTH INTERVALS WITHIN TTDYN
C     DSF        AVERAGING DEPTH (A) FOR SURFACE COMPOSITION
C     IQXN,IQXX LIMITING DEPTH INTERVALS FOR PROFILE OUTPUT
C                (IQXN = 0: ALL INTERVALS)
C     IMCP       COMPONENT FOR WHICH MOMENTS SHALL BE CALCULATED
C                (= 0: NO MOMENT CALCULATION)
C
C     FOLLOWING RECORDS (FORMAT 6F7.2,F7.3,E10.3,F5.2)
C     (ONE FOR EACH COMPONENT, FIRST FOR PROJECTILE):
C
C     ZZ         ATOMIC NUMBER
C     M          ATOMIC MASS
C     SBE        SURFACE BINDING ENERGY (EV)
C     BE         BINDING ENERGY (EV)
C     ED         DISPLACEMENT ENERGY (EV)
C     EF         CUTOFF ENERGY (EV)
C     QU         MAXIMUM ALLOWABLE ATOMIC FRACTION (PROJECTILE)
C                INITIAL ATOMIC FRACTION (TARGET;IQ0=0)
C     DNS0       ATOMIC DENSITY OF PURE COMPONENT (A-3)
C     CK         PROJECTILE ELECTRONIC STOPPING CORRECTION FACTOR
C
C     ADDITIONAL RECORDS IN CASE OF IQ0<0 (FORMAT 10F6.3)
C     (VECTOR INPUT):
C
C     ONE SET OF NQX LOCAL ATOMIC FRACTIONS FOR EACH TARGET
C     COMPONENT (EXCLUDING PROJECTILE)
```

```
C
C     ADDITIONAL RECORDS IN CASE OF IQ0>0 (FORMAT E10.3,4F6.3)
C     (LAYER INPUT):
C
C     ARBITRARY NR. OF RECORDS CONTAINING EACH
C     DMAX          MAX.DEPTH (A)
C     QU(2...NCP)   ATOMIC FRACTIONS (TARGET)
C
C
C
C     OUTPUT ON CHANNEL 7:
C
C
C     QUANTITIES AS FUNCTION OF FLUENCE:
C
C     1.RECORD: (FORMAT 7E11.4)
C     FLUC      PROJECTILE FLUENCE (A-2)
C     SRRC      SURFACE RECESSION (A)
C     REEM1     REEMITTED PROJECTILE FLUENCE (A-2)
C     CSF       AVERAGED ATOMIC SURFACE CONCENTRATIONS (2...5)
C
C     2.RECORD: (FORMAT 5E11.4)
C     FLIB      MOMENTS OF DEPTH DISTRIBUTION OF COMPONENT IMCP
C               (INTEGRAL(A-2), MEAN DEPTH(A), STD.DEV.(A),
C               SKEWNESS, KURTOSIS)
C
C     3.RECORD: (FORMAT 5E11.4)
C     SPYD      SPUTTERING YIELDS (1...5)
C
C     4.RECORD: (FORMAT 5E11.4)
C     ARD       AREAL DENSITIES (1...5)
C
C
C     PROFILES:
C
C     ONE RECORD FOR EACH DEPTH INTERVAL: (FORMAT 2X,2E11.4,5F6.3)
C     XXX       CENTRAL DEPTH (A)
C     DNS       TOTAL ATOMIC DENSITY (A-3)
C     QUX       RELATIVE ATOMIC FRACTIONS (1...NCP)
C
C
C     OUTPUT ON CHANNEL 17:
C
C     DEPOSITION PROFILES, NORMALIZED TO TARGET ATOM DENSITY
C     (CPTS.#JNRM...NCP); IN CASE OF DYNAMIC MODE, THE FINAL
C     DENSITY IS TAKEN
C
C     HEADLINE AND DATA PAIRS (FORMAT 2E15.6) IN CONSECUTIVE ORDER FOR
```

```
C
C     RANGE OF PROJECTILES (AT.CONC. VS. DEPTH/CM)
C     FRENKEL PAIRS OF TARGET (CPTS.#JFRP...NCP), AS CALCULATED
C       FROM PRIMARY ENERGY TRANSFERS ACCORDING TO MODIFIED
C       KINCHIN-PEASE MODEL WITH AVERAGED DISPLACEMENT ENERGY
C       (AT.CONC. VS. DEPTH/CM)
C     PROJECTILE ELECTRONIC ENERGY LOSS (EV/ATOM VS. DEPTH/CM)
C     PROJECTILE NUCLEAR ENERGY LOSS (EV/ATOM VS. DEPTH/CM)
C     PROJECTILE NUCLEAR LOSS INTO DAMAGE (EV/ATOM VS. DEPTH/CM)
C     PROJECTILE NUCLEAR LOSS INTO PHONONS (EV/ATOM VS. DEPTH/CM)
C     FRENKEL PAIRS OF INDIVIDUAL COMPONENTS (NCP DATA SETS)
C       (ATOMS SET IN MOTION ABOVE DISPLACEMENT THRESHOLD,
C       INCLUDING COLLISION CASCADES)
C
C
      DIMENSION EC(5,5),A(5,5),F(5,5),CK(5),SBE(5),EF(5),NCLR(500)
      DIMENSION IRP(500),IPL(500),DMGN(500),ER(600,2),ION(500)
      DIMENSION PHON(500),L(600,2),KO(600,5,2),RION(500)
      DIMENSION XR(600,2),YR(600,2),ZR(600,2)
      DIMENSION CSXR(600,2),CSYR(600,2),CSZR(600,2),SXR(600)
      DIMENSION ZZ(5),LABEL(600,2),FPKP(500),FACT(500)
      DIMENSION IBSP(5),EBSP(5),EPS0(5)
      DIMENSION ISPINP(5),ESPINP(5),ISPINS(5),ESPINS(5)
      DIMENSION ISPOP(5),ESPOP(5),ISPOS(5),ESPOS(5)
C
      DIMENSION QUX(500,5),XXX(500),DNS(500),XNO(501),QUX0(500,5)
      DIMENSION DEL(500,5),IXST(600,2),EORC(600,2)
      DIMENSION DNS0(5),BE(5),ED(5),QU(5),QUINP(5),ARD(5),QUXB(5)
      DIMENSION CSF(5),FLIB(5),IBSPO(5),SPYD(5),SSUM(5),QUXI(5)
      DIMENSION TITLE(16),BBR(500,5),BBRTOT(5)
      DIMENSION PR(600),X2(600),BR(600),EX1R(600),EX2R(600),EX3R(600)
      DIMENSION VR(600),V1R(600),C2R(600),S2R(600),STR(600)
      DIMENSION T(600),TS(600),DEERS(600),TAUR(600),CTR(600)
      DIMENSION PHIR(600,2),PSIR(600,2),ASIGTR(600),DEER(600),EPSR(600)
      DIMENSION CXR(600),CYR(600),CZR(600),SNXR(600,2)
      DIMENSION RRV(600),INOUT(600,2),IXRV(600),PMAXV(600),LMV(600,2)
      DIMENSION SQUXV(5,600),KL2(600),CUR(600)
      DIMENSION DNSOV(500),DXV(500),SUMV(500),CHAV(500),D1MXV(500)
      COMMON/A/M1,VELC,ZARG
      LOGICAL TEST(600)
C
      REAL MU(5,5),M(5),LM,KL(5,5),K(5),KOR(5,5),K23
      REAL M1,ION,NCLR,LMV
      REAL IONTOT,NCLTOT
C
      DATA PI/3.14159265/,SQ2PI/1.77245385/
      DATA QUX/2500*0./,IBSPO/5*0/,SPYD/5*0./,FLIB/5*0./,ARD/5*0./
      DATA IRP/500*0/,IPL/500*0/,DMGN/500*0./,AVEX/0./,AVEPL/0./
```

```
      DATA IB/0/,XSUM/0./,PLSUM/0./,IT/0/,EB/0./,ET/0./,IERR/1/
      DATA IONTOT/0./,NCLTOT/0./,PHOTOT/0./,DMGTOT/0./,FPKTOT/0./
      DATA X2SUM/0./,PL2SUM/0./,IBSP/5*0/,EBSP/5*0/,CSF/5*0./
      DATA ION/500*0./,NCLR/500*0./,BBR/2500*0./,PHON/500*0./
      DATA ISPINP/5*0/,ESPINP/5*0/,ISPINS/5*0/,ESPINS/5*0/,X3SUM/0./
      DATA ISPOP/5*0/,ESPOP/5*0/,ISPOS/5*0/,ESPOS/5*0/,X4SUM/0./
      DATA ICSUM/0/,ICSUM1/0/,FPKP/500*0./,BBRTOT/5*0./
      DATA MAXA/0/,NALL/0/
      DATA AVSO/3H3.1/
      DATA NQXM,NCPM,MAXMAX,MAXSD/500,5,600,100/
C
       IO = 6
       IO1 = 7
       IO2 = 17
C
C     READ INPUT DATA
C
      READ(5,4195)TITLE
4195  FORMAT(16A4)
      READ(5,4005)NH,IDOUT,IQOUT,NCP,IDREL,IQ0,IRC0,IRAND,JSP1,JSP2,
     CJFRP,JNRM
4005  FORMAT(I10,11I5)
      READ(5,4015)FLC,E0,X0,ALPHA,INEL,INELR,IWC,IWCR,SHTH
4015  FORMAT(E10.3,3F10.2,4I5,F10.2)
      READ(5,4025)TT,TTDYN,NQX,DSF,IQXN,IQXX,IMCP
4025  FORMAT(2E10.3,I5,E10.3,3I5)
      DO 4010 JP=1,NCP
4010  READ(5,4035)ZZ(JP),M(JP),SBE(JP),BE(JP),ED(JP),EF(JP),QU(JP)
     C,DNS0(JP),CK(JP)
4035  FORMAT(6F7.2,F7.3,E10.3,F5.2)
C
C     SET INITIAL ATOMIC FRACTIONS AND DENSITIES FOR
C     EQUIDISTANT INTERVALS
C
      DQX = TTDYN/NQX
      IF(IQ0)4890,4020,4900
4890  DO 4030 JP=2,NCP
      READ(5,4045)(QUX(MM,JP),MM=1,NQX)
4045  FORMAT(10F6.3)
4030  QUINP(JP) = 0.
      GOTO 4040
4900  DO 4910 JP=2,NCP
4910  QUINP(JP) = 0.
      DMAX = 0.
      DO 4920 MM=1,NQX
      SUM = (MM-.5)*DQX
4940  IF(SUM.LE.DMAX) GOTO 4930
      READ(5,4915)DMAX,(QU(JP),JP=2,NCP)
```

```
4915  FORMAT(E10.3,4F6.3)
      GOTO 4940
4930  DO 4920 JP=2,NCP
4920  QUX(MM,JP) = QU(JP)
      GOTO 4040
4020  DO 4050 JP=2,NCP
      QUINP(JP) = QU(JP)
      DO 4050 MM=1,NQX
4050  QUX(MM,JP) = QU(JP)
4040  QUINP(1) = QU(1)
      IF(IQO.EQ.0) GOTO 5050
      DO 5060 JP=2,NCP
      DO 5060 MM=1,NQX
5060  QUXO(MM,JP) = QUX(MM,JP)
5050  QU1MX = QU(1)
      DO 4100 MM=1,NQX
      XXX(MM) = (MM-.5)*DQX
      XNO(MM) = (MM-1)*DQX
      SUM = 0.
      DNS(MM) = 0.
      DO 4070 JP=2,NCP
      SUM = SUM+QUX(MM,JP)
4070  DNS(MM) = DNS(MM)+QUX(MM,JP)/DNSO(JP)
      DNS(MM) = 1./(DNS(MM)+(1.-SUM)/DNSO(1))
4100  QUX(MM,1) = 1.-SUM
      XNO(NQX+1) = TTDYN
      SUM = 0.
      DO 4230 JP=2,NCP
      QUXB(JP) = QUX(NQX,JP)
4230  SUM = SUM+QUXB(JP)
      QUXB(1) = 1.-SUM
      DNSB = DNS(NQX)
C
C     INITIAL OUTPUT OF INTEGRAL DATA
C
      IF(IQXN.LE.0) GOTO 4870
      NQOUT = IQXX-IQXN+1
      GOTO 4880
4870  IQXN = 1
      IQXX = NQX
      NQOUT = NQX
4880  SRRC = 0.
      FLUC = 0.
      IF(IDOUT.LE.0.OR.IDREL.NE.0) GOTO 2220
      AMM = 0.
      DO 4060 JP=1,NCP
      CSF(JP) = 0.
4060  ARD(JP) = 0.
```

```
      DO 4730 MM=1,NQX
      SUM = 0.
      DO 4740 JP=2,NCP
4740  SUM = SUM+QUX(MM,JP)
      DO 4080 JP=1,NCP
4080  ARD(JP) = ARD(JP)+QUX(MM,JP)*DQX*DNS(MM)
      IF(XNO(MM).GE.DSF) GOTO 4730
      DAM = 1.
      IF(XNO(MM+1).LE.DSF) GOTO 4750
      DAM = (DSF-XNO(MM))/DQX
4750  AMM = AMM+DAM
      DO 4110 JP = 2,NCP
4110  CSF(JP) = CSF(JP)+QUX(MM,JP)/SUM*DAM
4730  CONTINUE
      IF(AMM.LE.0) GOTO 4440
      DO 4450 JP=2,NCP
4450  CSF(JP) = CSF(JP)/AMM
4440  IF(IMCP.LE.0) GOTO 4960
      DO 4970 MM=1,NQX
      FLIB(1) = FLIB(1)+QUX(MM,IMCP)*DQX*DNS(MM)
4970  FLIB(2) = FLIB(2)+QUX(MM,IMCP)*XXX(MM)*DQX*DNS(MM)
      IF(FLIB(1).LE.0.) GOTO 4960
      FLIB(2) = FLIB(2)/FLIB(1)
      DO 4980 MM=1,NQX
      SUM = QUX(MM,IMCP)*DQX*DNS(MM)*(XXX(MM)-FLIB(2))**2
      FLIB(3) = FLIB(3)+SUM
      FLIB(4) = FLIB(4)+SUM*(XXX(MM)-FLIB(2))
4980  FLIB(5) = FLIB(5)+SUM*(XXX(MM)-FLIB(2))**2
      IF(FLIB(3).LT.1.E-10*FLIB(2)) GOTO 5030
      FLIB(3) = SQRT(FLIB(3)/FLIB(1))
      FLIB(4) = FLIB(4)/FLIB(3)**3
      FLIB(5) = FLIB(5)/FLIB(3)**4-3.
      GOTO 4960
5030  FLIB(3) = 0.
      FLIB(4) = 0.
      FLIB(5) = 0.
4960  WRITE(IO1,2025)
2025  FORMAT('DYNAMIC COMPOSITION TRIM PROGRAM')
      WRITE(IO1,2055)NH,IDOUT,IQOUT,NCP,NQOUT
2055  FORMAT(5I10,5X,'TRIDYN31')
      WRITE(IO1,2035)FLUC,SRRC,FLUC,(CSF(JP),JP=2,NCPM),FLIB,SPYD,ARD
2035  FORMAT(7E11.4,3(/5E11.4))
C
C     INITIAL OUTPUT OF PROFILES
C
      IF(IQOUT.LE.0) GOTO 2220
      DO 4090 MM=IQXN,IQXX
4090  WRITE(IO1,2045)XXX(MM),DNS(MM),(QUX(MM,JP),JP=1,NCP)
```

```
2045  FORMAT(2X,2E11.4,5F6.3)
C
C     SET UNIVERSAL AND INITIAL QUANTITIES
C
2220  CHAMAX = 0.
      SRRCN = 0.
      REEM1 = 0.
      IF(QU1MX.LT.0..OR.QU1MX.GT.1.) QU1MX = 1.
      IF(JNRM.LE.0.OR.JNRM.GT.NCP) JNRM = NCP
      IF(JFRP.LE.0.OR.JFRP.GT.NCP) JFRP = NCP
      JSP1I = JSP1
      IF(JSP1.LE.0) JSP2 = 0
      IF(JSP1.LE.0) JSP1 = NCP+1
      IPREC = 0
      KK1 = 4-IWC
      KK2 = 4-IWCR
      ALPHA = CVMGT(.001,ALPHA,ALPHA.EQ.0.)
      ALPHA = CVMGT(179.999,ALPHA,ALPHA.EQ.180.)
      ALFA=ALPHA/57.295779
      DO 102 I=1,NCP
      DO 102 J=1,NCP
      MU(I,J)=M(I)/M(J)
      EC(I,J)=4.*MU(I,J)/(1.+MU(I,J))**2
      A(I,J)=.529*.8853/(ZZ(I)**.5+ZZ(J)**.5)**(2./3.)
      F(I,J)=A(I,J)*M(J)/(ZZ(I)*ZZ(J)*14.4*(M(I)+M(J)))
      KL(I,J)=1.212*ZZ(I)**(7./6.)*ZZ(J)/((ZZ(I)**(2./3.)+ZZ(J)**(2./3.
     ?))**1.5*SQRT(M(I)))
      KOR(I,J)=.03892*KL(I,J)/(PI*A(I,J)**2)
  102 CONTINUE
      Z1=ZZ(1)
      M1=M(1)
      DO 104 J=1,NCP
      K(J)=CK(J)*KL(1,J)
  104 EPSO(J)=ABS(E0)*F(1,J)
      ANFANG = RANSET(IRAND)
      IF(E0.GE.0.) GOTO 105
      TI = -E0
      ZARG = SQRT(TI/2./M1)
      VELC = SHTH/M1
C
C     PROJECTILE HISTORY LOOP
C
105   IH = 0
10    IH = IH+1
      IF(IH.GT.NH) GOTO 18
C
C     PROJECTILE START
C
```

```
      DO 2070 JP=1,NCP
      DO 2070 MM=1,NQX
2070  DEL(MM,JP) = 0.
      SU = DNS(1)**(-1./3.)/SQ2PI*2.
      XC = CVMGT(X0,-SU,X0.GT.0.)
      IC=0
      IC1=0
      PL = 0.
      NREC1=1
      IF(E0.GE.0.) GOTO 106
C
C     MAXWELLIAN ENERGY-ANGLE DISTRIBUTION
C
      CALL MXVELO(E,COSX,COSY,COSZ,SINE)
      GOTO 107
106   E = E0
      IF(ALPHA.LT.0.) GOTO 108
      COSX = COS(ALFA)
      COSY = SIN(ALFA)
      COSZ = 0.
      SINE = COSY
      GOTO 107
108   IF(ALPHA.NE.-2.) GOTO 109
C
C     2-DIM COSINE ANGLE DISTRIBUTION
C
      RPHI = RANF()
      RTHETA = RANF()
      COSX = SQRT(RTHETA)
      SINE = SQRT(1.-RTHETA)
      COSY = SINE*COS(2.*PI*RPHI)
      COSZ = SINE*SIN(2.*PI*RPHI)
      GOTO 107
C
C     RANDOM ANGLE DISTRIBUTION
C
109   RPHI = RANF()
      RTHETA = RANF()
      COSX = 1.-RTHETA
      IF(X0.GT.0.) COSX = COSX-RTHETA
      SINE = SQRT(1.-COSX**2)
      COSY = SINE*COS(2.*PI*RPHI)
      COSZ = SINE*SIN(2.*PI*RPHI)
C
C     EXTERNAL START
C
107   IF(X0.GT.0.) GOTO 110
      SINA = SINE
```

```
      COSX = SQRT((E*COSX**2+SBE(1))/(E+SBE(1)))
      SINE = SQRT(1.-COSX**2)
      COSY = COSY*SINE/SINA
      COSZ = COSZ*SINE/SINA
      E = E+SBE(1)
C
C     PROJECTILE START INTERVAL
C
110   IX = ISRCHFGE(NQX+1,XNO(1),1,XC)-1
      IX = MAXO(IX,1)
      IF(IX.LE.NQX) GOTO 2130
2140  WRITE(IO,2075)IH,IC,X,E,IERR,XR(IERR,2),ER(IERR,2)
2075  FORMAT(5X,'IH=',I7,'    IC=',I5,'     X=',E11.4,'     E=',E11.4/
     C18X,'IR=',I5,'    XR=',E11.4,'    ER=',E11.4)
      WRITE(IO,2095)
2095  FORMAT(5X,'PARTICLE RANGE EXCEEDS DYNAMIC COMPOSITION RANGE'/
     C5X,'----- INCREASE TTDYN')
      STOP
2130  LM = DNS(IX)**(-1./3.)
C
C     LOCUS OF FIRST COLLISION
C
      RA = 1.
      IF(XO.LE.O.) RA = RANF()
      X = XC+LM*COSX*RA
      Y = LM*COSY*RA
      Z = LM*COSZ*RA
      GOTO 2
C
C     COLLISION LOOP
C
C     MOVE PROJECTILES
C
    1 X=X+LM*COSX
      Y=Y+LM*COSY
      Z=Z+LM*COSZ
C
C     STORE DIRECTIONS
C
2     CX = COSX
      CY = COSY
      CZ = COSZ
      SX = SINE
      EX1 = 0.
      DEES = 0.
      DENS = 0.
C
C     DEPTH INTERVAL OF COLLISION
```

```
C
      IX = ISRCHFGE(NQX+1,XNO(1),1,X)-1
      IX = MAXO(IX,1)
      IF(IX.GT.NQX) GOTO 2140
C
C     COLLISION PARAMETERS
C
      LM = DNS(IX)**(-1./3.)
      ASIG = LM*DNS(IX)
      PMAX = LM/SQ2PI
      K23 = 0.
      DO 4120 JP=1,NCP
4120  K23 = K23+K(JP)*QUX(IX,JP)
C
C     WEAK COLLISION LOOP
C
      DO 245 KK=KK1,4
      TAU = 0.
      DEN = 0.
C
C     SPECIES OF COLLISION PARTNER
C
      RR = RANF()
      SUM = 1.-QUX(IX,1)
      DO 4130 J=1,NCP-1
      IF(RR.GT.SUM) GOTO 4140
4130  SUM = SUM-QUX(IX,J+1)
      J = NCP
4140  LABEL(NREC1,1)=J
      JPKO = J
C
C     AZIMUTHAL ANGLE, IMPACT PARAMETER, REDUCED ENERGY
C
      PHI=2.*PI*RANF()
      P=PMAX*SQRT(RANF()+4.-KK)
      EPS=E*F(1,J)
      IF(KK.LT.4.AND.EPS.GT.1.E-2) GOTO 245
C
C     POSITION OF TARGET ATOM
C
      X1=X-P*COS(PHI)*SX
      IF(X1.LT.0.) GOTO 245
C
C      MAGIC (DETERMINATION OF SCATTERING ANGLE : ION - TARGET ATOM :
C      KR-C POTENTIAL)
C
      B = P/A(1,J)
      R=B
```

```
      RR=ALOG(.35/(EPS*B))*3.33333333333
      IF (RR.LT.B) GO TO 121
      RR=ALOG(.35/(EPS*RR))*3.3333333333
      IF (RR.LT.B) GO TO 121
      R=RR
  121 EX1=EXP(-.279*R)
      EX2=EXP(-.637*R)
      IF(EX2-1.E-10)122,123,123
  123 CONTINUE
      EX3=EXP(-1.919*R)
      GO TO 124
  122 EX3=0.0
  124 CONTINUE
      RRR1 = 1.0/R
      V=(.191*EX1+.474*EX2+.335*EX3)*RRR1
      FR=B*B*RRR1+V*R/EPS-R
      V1=-(V+.0531865*EX1+.30181*EX2+.6437*EX3)*RRR1
      FR1=-B*B*RRR1**2+(V+V1*R)/EPS-1.
      Q=FR/FR1
      R=R-Q
      IF (ABS(Q/R).GT..001) GO TO 121
      ROC=-2.*(EPS-V)/V1
      SQE=SQRT(EPS)
      CC=(.235800+SQE)/(.126000+SQE)
      AA=2.*EPS*(1.+(1.0144/SQE))*B**CC
      FF=(SQRT(AA**2+1.)-AA)*((69350.+EPS)/(83550.+EPS))
      DELTA=(R-B)*AA*FF/(FF+1.)
      C=(B+DELTA+ROC)/(R+ROC)
      C2=AMIN1(1.0,C*C)
      S2=1.-C2
C
C     ENERGY TRANSFER, LOCAL INELASTIC ENERGY LOSS, SCATTERING ANGLE
C
      DEN = EC(1,J)*S2*E
      DENS = DENS+DEN
      IF(DEN.GT.ED(J)) IC1 = IC1+1
      DEEOR = CVMGT(0.,CK(J)*KOR(1,J)*SQRT(E)*EX1,INEL.EQ.1)
      DEES = DEES+DEEOR
      TAU = R*A(1,J)*SQRT(S2)
      CT=2.*C2-1.
      ST=SQRT(1.-CT*CT)
      CU = CT+MU(1,J)
      IF(ABS(CU).LT.1.E-8) CU = 1.E-8
      PSI = ATAN2(ST,CU)
      IF(PSI.LT.0.) PSI = PSI+PI
C
C     NEW DIRECTIONS
C
```

```
      CALL DIRCOS(COSX,COSY,COSZ,SINE,PSI,PHI)
C
C     END OF WEAK COLLISION LOOP
C
245   CONTINUE
C
C     BOND BREAKING
C
      IF(DEN.LE.ED(J)) GOTO 128
      BBR(IX,J) = BBR(IX,J)+1.
      BBRTOT(J) = BBRTOT(J)+1.
C
C     GENERATION OF PRIMARY KNOCKON
C
128   IF(IDREL.LT.0) GOTO 127
      IF(DEN.LE.BE(J)) GOTO 127
      IF(J.GE.JSP1.AND.J.LE.JSP2) GOTO 127
      ER(NREC1,1)=DEN-BE(J)
      IF(ER(NREC1,1).LE.EF(J)) GOTO 127
      LMV(NREC1,1)=LM
      CPHI=COS(PHI)
      SPHI=SIN(PHI)
      XR(NREC1,1)=X1
      YR(NREC1,1)=Y-P*(SPHI*CZ-CPHI*CY*CX)/SX
      ZR(NREC1,1)=Z+P*(SPHI*CY+CPHI*CZ*CX)/SX
      CSXR(NREC1,1)=CX
      CSYR(NREC1,1)=CY
      CSZR(NREC1,1)=CZ
      SNXR(NREC1,1)=SX
      PHIR(NREC1,1)=PHI-PI
      CT = AMIN1(CT,.99999999)
      PSIR(NREC1,1)=ATAN2(ST,1.-CT)
      IXST(NREC1,1) = IX
      L(NREC1,1) = X1+1.
      KO(NREC1,J,1)=1
      EORC(NREC1,1) = ER(NREC1,1)
      INOUT(NREC1,1)=SIGN(1.,CX)
      DEL(IX,J) = DEL(IX,J)-1.
      NREC1=NREC1+1
      IF(NREC1.LE.MAXMAX) GOTO 127
75    WRITE(IO,130)
130   FORMAT(5X,'RECOIL STORAGE CAPACITY EXCEEDED')
      STOP
C
C     TOTAL INELASTIC ENERGY LOSS
C
127   ASIGT = ASIG-TAU*DNS(IX)
      GOTO(15,16,17)INEL
```

```
15      DEE = CVMGT(0.,K23*ASIGT*SQRT(E),X.LT.0.)
        GOTO 7
16      DEE = DEES
        GOTO 7
17      DEE = CVMGT(DEES,.5*(K23*ASIGT*SQRT(E)+DEES),X.LT.0.)
C
C       COLLISION COUNTER
C
      7 IF(DENS.GT.0.) IC = IC+1
C
C       PROJECTILE ENERGY AND ENERGY DEPOSITION FUNCTIONS
C
        IXI = INT(X/DQX)+1
        IF(IXI.LE.0) IXI = 1
        ION(IXI) = ION(IXI)+DEE
        IONTOT = IONTOT+DEE
        NCLR(IXI) = NCLR(IXI)+DENS
        NCLTOT = NCLTOT+DENS
        PHON(IXI) = PHON(IXI)+DENS-DEN
        PHOTOT = PHOTOT+DENS-DEN
        IF(DEN.LE.ED(JPKO)) GOTO 28
        DMGN(IXI) = DMGN(IXI)+DEN
        DMGTOT = DMGTOT+DEN
        GOTO 4860
28      PHON(IXI) = PHON(IXI)+DEN
        PHOTOT = PHOTOT+DEN
4860    IF(JPKO.LT.JFRP) GOTO 29
        EDM = 0.
        SUM = 0.
        DO 4850 JP = JFRP,NCP
        SUM = SUM+QUX(IXI,JP)
4850    EDM = EDM+QUX(IXI,JP)/ED(JP)
        EDM = SUM/EDM
        IF(DEN.LE.EDM) GOTO 29
        IF(DEN.GT.2.5*EDM) GOTO 4840
        FPKP(IXI) = FPKP(IXI)+1.
        FPKTOT = FPKTOT+1.
        GOTO 29
4840    FPKP(IXI) = FPKP(IXI)+.35*DEN/EDM
        FPKTOT = FPKTOT+.35*DEN/EDM
C
C       ENERGY AND DEFLECTION POINT OF PROJECTILE
C
29      E = E-DEE
        X=X-TAU*CX
        Y=Y-TAU*CY
        Z=Z-TAU*CZ
        PL=PL+LM-TAU
```

```
C
C     PARTICLE STOPPED, REFLECTED OR TRANSMITTED
C
      IF(X.LT.-SU) GOTO 8
      IF(X.GT.TT) GOTO 9
      IF(E-DENS.LT.EF(1)) GOTO 4
      GOTO 5
    8 ENO=E*COSX**2
      IF(ENO.GT.SBE(1)) GOTO 24
C
C     BACKREFLECTED PROJECTILES
C
      X = -SU
      COSX=-COSX
      GOTO 5
C
C     BACKSCATTERED PROJECTILES
C
24    ES = E-SBE(1)
      IB=IB+1
      EB = EB+ES
      GOTO 6
C
C     TRANSMITTED PROJECTILES
C
9     IT=IT+1
      ET=ET+E
      GOTO 6
C
C     PROJECTILE STOPPED
C
4     DEL(IX,1) = DEL(IX,1)+1.
      IXI = INT(X/DQX)+1
      IF(IXI.LE.0) IXI = 1
      IRP(IXI) = IRP(IXI)+1
      IP=INT(PL/DQX+1.)
      IF(IP.GT.NQX) IP=NQX
      IPL(IP)=IPL(IP)+1
      IF(X.LT.0.) X = 0.
      XSUM = XSUM+X
      X2SUM = X2SUM+X*X
      X3SUM = X3SUM+X**3
      X4SUM = X4SUM+X**4
      PLSUM=PLSUM+PL
      PL2SUM=PL2SUM+PL**2
      ICSUM=ICSUM+IC
      ICSUM1=ICSUM1+IC1
      GOTO 6
```

```
C
C     ELEASTIC ENERGY LOSS
C
5     E = E-DENS
      GOTO 1
C
C     END OF PROJECTILE SECTION
C
6     NREC1=NREC1-1
      IF(NREC1.LE.0) GOTO 10
C
C     RECOIL ATOM SECTION
C
      NREC2=0
73    IF(NREC1.LE.0) GOTO 74
C
C     DIRECTIONS OF NEW RECOILS (LIST 1)
C
      CALL DIRCOSV(CSXR(1,1),CSYR(1,1),CSZR(1,1),SNXR(1,1),
     CPSIR(1,1),PHIR(1,1),NREC1)
C
C     MOVE NEW RECOILS (LIST 1) TO LIST 2
C
      DO 91 IREC1=1,NREC1
      IREC=IREC1+NREC2
      ER(IREC,2)=ER(IREC1,1)
      EORC(IREC,2) = EORC(IREC1,1)
      XR(IREC,2)=XR(IREC1,1)
      YR(IREC,2)=YR(IREC1,1)
      ZR(IREC,2)=ZR(IREC1,1)
      CSXR(IREC,2)=CSXR(IREC1,1)
      CSYR(IREC,2)=CSYR(IREC1,1)
      CSZR(IREC,2)=CSZR(IREC1,1)
      SNXR(IREC,2)=SNXR(IREC1,1)
      L(IREC,2)=L(IREC1,1)
      LMV(IREC,2)=LMV(IREC1,1)
      LABEL(IREC,2)=LABEL(IREC1,1)
      IXST(IREC,2)=IXST(IREC1,1)
      KO(IREC,LABEL(IREC1,1),2)=KO(IREC1,LABEL(IREC1,1),1)
      INOUT(IREC,2)=INOUT(IREC1,1)
   91 CONTINUE
      NREC2=NREC2+NREC1
      MAXA=MAX0(MAXA,NREC2)
      NREC1=0
74    NALL=NALL+NREC2
C
C     PROCESS THE PARTICLES IN LIST 2
C
```

```
C     MOVE PARTICLES
C
      DO 60 IREC1=1,NREC2
      XR(IREC1,2)=XR(IREC1,2)+LMV(IREC1,2)*CSXR(IREC1,2)
      YR(IREC1,2)=YR(IREC1,2)+LMV(IREC1,2)*CSYR(IREC1,2)
      ZR(IREC1,2)=ZR(IREC1,2)+LMV(IREC1,2)*CSZR(IREC1,2)
   60 CONTINUE
C
C     STORE DIRECTIONS
C
      DO 81 IREC1=1,NREC2
      CXR(IREC1)=CSXR(IREC1,2)
      CYR(IREC1)=CSYR(IREC1,2)
      CZR(IREC1)=CSZR(IREC1,2)
      SXR(IREC1)=SNXR(IREC1,2)
      DEERS(IREC1)=0.
      TS(IREC1)=0.
   81 CONTINUE
C
C     DEPTH INTERVAL OF COLLISION
C
      DO 84 IREC1=1,NREC2
      IXRV(IREC1) = ISRCHFGE(NQX+1,XNO(1),1,XR(IREC1,2))-1
      IXRV(IREC1) = MAX0(IXRV(IREC1),1)
84    TEST(IREC1) = IXRV(IREC1).GT.NQX
      IERR = ILLZ(NREC2,TEST,1)
      IF(IERR.EQ.NREC2) GOTO 80
      IERR = IERR+1
      GOTO 2140
C
C     DEPTH-DEPENDENT PARAMETERS
C
80    DO 85 IREC1=1,NREC2
      LMV(IREC1,2) = DNS(IXRV(IREC1))**(-1./3.)
      PMAXV(IREC1) = LMV(IREC1,2)/SQ2PI
85    KL2(IREC1) = 0.
      DO 4150 JP=1,NCP
      DO 4150 IREC1=1,NREC2
      J = LABEL(IREC1,2)
      IXRC=IXRV(IREC1)
      KL2(IREC1)=KL2(IREC1)+KL(J,JP)*QUX(IXRC,JP)
4150  CONTINUE
C
C     WEAK COLLISION LOOP
C
      DO 235 KK=KK2,4
C
C     SPECIES OF COLLISION PARTNER
```

```
C
      IF(NCP.GT.1) GOTO 82
      DO 83 IREC1=1,NREC2
83    LABEL(IREC1,1) = 1
      GOTO 90
82    DO 86 IREC1=1,NREC2
      IXRC = IXRV(IREC1)
86    SQUXV(1,IREC1) = QUX(IXRC,1)
      IF(NCP.LE.2) GOTO 87
      DO 88 JP=2,NCP-1
      DO 88 IREC1=1,NREC2
      IXRC = IXRV(IREC1)
88    SQUXV(JP,IREC1) = SQUXV(JP-1,IREC1)+QUX(IXRC,JP)
87    DO 89 IREC1=1,NREC2
      SQUXV(NCP,IREC1) = 1.
89    LABEL(IREC1,1) = ISRCHFGE(NCP,SQUXV(1,IREC1),1,RANF())
C
C     AZIMUTHAL ANGLE, IMPACT PARAMETER, REDUCED ENERGY
C
90    DO 236 IREC1=1,NREC2
      PHIR(IREC1,2)=2.*PI*RANF()
      PR(IREC1)=PMAXV(IREC1)*SQRT(RANF()+4.-KK)
      X2(IREC1)=XR(IREC1,2)-PR(IREC1)*COS(PHIR(IREC1,2))*SXR(IREC1)
      PR(IREC1)=CVMGT(1.E10,PR(IREC1),X2(IREC1).LT.0.)
      BR(IREC1)=PR(IREC1)/A(LABEL(IREC1,2),LABEL(IREC1,1))
      EPSR(IREC1) = ER(IREC1,2)*F(LABEL(IREC1,2),LABEL(IREC1,1))
  236 CONTINUE
C
C     'MAGIC' CALCULATION OF POLAR DEFLECTION
C
      CALL SCOPY(NREC2,BR,1,RRV,1)
      IVMIN=1
      IVMAX=NREC2
  205 DO 206 IV=IVMIN,IVMAX
      EX1R(IV)=EXP(-.279*RRV(IV))
      EX2R(IV)=EXP(-.637*RRV(IV))
      EX3R(IV)=EXP(-1.919*RRV(IV))
      RRR1=1./RRV(IV)
      VR(IV)=(.191*EX1R(IV)+.474*EX2R(IV)+.335*EX3R(IV))*RRR1
      FR=BR(IV)*BR(IV)*RRR1+VR(IV)*RRV(IV)/EPSR(IV)-RRV(IV)
      V1R(IV)=-(VR(IV)+.0531865*EX1R(IV)+.30181*EX2R(IV)+
     1       .6437*EX3R(IV))*RRR1
      FR1=-BR(IV)*BR(IV)*RRR1*RRR1+(VR(IV)+V1R(IV)*RRV(IV))/
     1   EPSR(IV)-1.
      Q=FR/FR1
      RRV(IV)=RRV(IV)-Q
      TEST(IV)=ABS(Q/RRV(IV)).GT.0.001
  206 CONTINUE
```

```
C     GET MAX AND MIN INDEX OF TEST FAILURES
      IVMIN=IVMIN+ILLZ(IVMAX-IVMIN+1,TEST(IVMIN),1)
      IF(IVMIN.GT.IVMAX) GO TO 207
      IVMAX=IVMAX-ILLZ(IVMAX-IVMIN+1,TEST(IVMIN),-1)
      IF(IVMIN.GT.IVMAX) GO TO 207
      GO TO 205
  207 DO 208 IV=1,NREC2
      ROCINV=-.5*V1R(IV)/(EPSR(IV)-VR(IV))
      SQE=SQRT(EPSR(IV))
      CC=(.235800+SQE)/(.126000+SQE)
      AA=2.*EPSR(IV)*(1.+(1.0144/SQE))*BR(IV)**CC
      FF=(SQRT(AA*AA+1.)-AA)*((69350.+EPSR(IV))/(83550.+EPSR(IV)))
      DELTA=(RRV(IV)-BR(IV))*AA*FF/(FF+1.)
      C=(ROCINV*(BR(IV)+DELTA)+1.)/(ROCINV*RRV(IV)+1.)
      C2R(IV)=AMIN1(1.0,C*C)
  208 S2R(IV)=1.-C2R(IV)
C
C     ENERGY TRANSFER, LOCAL ELECTRONIC ENERGY LOSS, SCATTERING ANGLE
C
      DO 237 IREC1=1,NREC2
      T(IREC1)=ER(IREC1,2)*S2R(IREC1)*EC(LABEL(IREC1,2),LABEL(IREC1,1))
      TS(IREC1)=TS(IREC1)+T(IREC1)
      DEEROR=CVMGT(0.,KOR(LABEL(IREC1,2),LABEL(IREC1,1))
     C*SQRT(ER(IREC1,2))*EX1R(IREC1),INELR.EQ.1)
      DEERS(IREC1)=DEERS(IREC1)+DEEROR
      TAUR(IREC1)=RRV(IREC1)*A(LABEL(IREC1,2),LABEL(IREC1,1))
     C*SQRT(S2R(IREC1))
      CTR(IREC1)=C2R(IREC1)+C2R(IREC1)-1.
      STR(IREC1)=SQRT(1.-CTR(IREC1)*CTR(IREC1))
      CUR(IREC1) = CTR(IREC1)+MU(LABEL(IREC1,2),LABEL(IREC1,1))
      CUR(IREC1) = CVMGT(CUR(IREC1),1.E-8,ABS(CUR(IREC1)).GE.1.E-8)
      PSIR(IREC1,2) = ATAN2(STR(IREC1),CUR(IREC1))
      PSIR(IREC1,2) = CVMGT(PSIR(IREC1,2),PSIR(IREC1,2)+PI,PSIR(IREC1,2)
     C.GE.0.)
  237 CONTINUE
C
C     NEW DIRECTIONS OF OLD RECOIL
C
      CALL DIRCOSV(CSXR(1,2),CSYR(1,2),CSZR(1,2),SNXR(1,2),
     1            PSIR(1,2),PHIR(1,2),NREC2)
  235 CONTINUE
C
C     BOND BREAKING
C
      DO 240 IREC1=1,NREC2
      IF(T(IREC1).LE.ED(LABEL(IREC1,1))) GO TO 240
      J = LABEL(IREC1,1)
      IXRC = IXRV(IREC1)
```

```
      BBR(IXRC,J) = BBR(IXRC,J)+1.
      BBRTOT(J) = BBRTOT(J)+1.
240   CONTINUE
C
C     CREATE SECONDARY KNOCK-ON ATOMS (LIST 1)
C
      DO 246 IREC1=1,NREC2
      IF(T(IREC1).LE.BE(LABEL(IREC1,1))) GO TO 246
      IF(T(IREC1)-BE(LABEL(IREC1,1)).LE.EF(LABEL(IREC1,1))) GO TO 246
      IF(LABEL(IREC1,1).GE.JSP1.AND.LABEL(IREC1,1).LE.JSP2) GOTO 246
      NREC1=NREC1+1
      LMV(NREC1,1)=LMV(IREC1,2)
      ER(NREC1,1)=T(IREC1)-BE(LABEL(IREC1,1))
      CPR=COS(PHIR(IREC1,2))
      SPR=SIN(PHIR(IREC1,2))
      XR(NREC1,1)=X2(IREC1)
      YR(NREC1,1)=YR(IREC1,2)-PR(IREC1)*(SPR*CZR(IREC1)-
     1             CPR*CYR(IREC1)*CXR(IREC1))/SXR(IREC1)
      ZR(NREC1,1)=ZR(IREC1,2)+PR(IREC1)*(SPR*CYR(IREC1)+
     1             CPR*CXR(IREC1)*CZR(IREC1))/SXR(IREC1)
      CSXR(NREC1,1)=CXR(IREC1)
      CSYR(NREC1,1)=CYR(IREC1)
      CSZR(NREC1,1)=CZR(IREC1)
      SNXR(NREC1,1)=SXR(IREC1)
      PHIR(NREC1,1)=PHIR(IREC1,2)-PI
      CTR(NREC1)=AMIN1(CTR(IREC1),.99999999)
      PSIR(NREC1,1)=ATAN2(STR(IREC1),1.-CTR(NREC1))
      IXST(NREC1,1)=IXRV(IREC1)
      L(NREC1,1)=XR(NREC1,1)+1.
      LABEL(NREC1,1) = LABEL(IREC1,1)
      KO(NREC1,LABEL(IREC1,1),1)=0
      EORC(NREC1,1) = ER(NREC1,1)
      INOUT(NREC1,1)=INOUT(IREC1,2)
      DEL(IXRV(IREC1),LABEL(IREC1,1))=DEL(IXRV(IREC1),LABEL(IREC1,1))-1.
  246 CONTINUE
C
C     INELASTIC ENERGY LOSS
C
      DO 238 IREC1=1,NREC2
      IXRC=IXRV(IREC1)
      ASIGTR(IREC1)=(LMV(IREC1,2)-TAUR(IREC1))*DNS(IXRC)
  238 CONTINUE
      GO TO(115,116,117),INELR
  115 DO 241 IREC1=1,NREC2
      DEER(IREC1)=CVMGT(0.,KL2(IREC1)*ASIGTR(IREC1)*SQRT(ER(IREC1,2)),
     1                   XR(IREC1,2).LT.0.)
  241 CONTINUE
      GO TO 242
```

```
  116 DO 243 IREC1=1,NREC2
      DEER(IREC1)=DEERS(IREC1)
  243 CONTINUE
      GO TO 242
  117 DO 244 IREC1=1,NREC2
      DEER(IREC1)=CVMGT(DEERS(IREC1),.5*(KL2(IREC1)
     1            *ASIGTR(IREC1)*SQRT(ER(IREC1,2))+DEERS(IREC1)),
     2            XR(IREC1,2).LT.0.)
  244 CONTINUE
  242 CONTINUE
C
C     FINAL ENERGY AND POSITION OF OLD RECOIL
C
      DO 253 IREC1=1,NREC2
      ER(IREC1,2)=ER(IREC1,2)-DEER(IREC1)
      XR(IREC1,2)=XR(IREC1,2)-TAUR(IREC1)*CXR(IREC1)
      YR(IREC1,2)=YR(IREC1,2)-TAUR(IREC1)*CYR(IREC1)
      ZR(IREC1,2)=ZR(IREC1,2)-TAUR(IREC1)*CZR(IREC1)
      TEST(IREC1)=ER(IREC1,2)-TS(IREC1).LE.EF(LABEL(IREC1,2))
     C.OR.XR(IREC1,2).LT.-SU.OR.XR(IREC1,2).GT.TT
  253 CONTINUE
C
C     ANY RECOIL ATOM SLOWED DOWN, TRANSMITTED OR SPUTTERED ?
C
      IVMIN=1+ILLZ(NREC2,TEST,1)
      IF(IVMIN.GT.NREC2) GO TO 247
      IVMAX=NREC2-ILLZ(NREC2,TEST,-1)
      IREC1=IVMIN
248   IF(IREC1.GT.IVMAX.OR.IREC1.GT.NREC2) GOTO 247
      IF(.NOT.TEST(IREC1)) GOTO 249
      IF(XR(IREC1,2).LT.(-SU)) GO TO 251
      IF(XR(IREC1,2).GT.TT) GO TO 255
      IF(ER(IREC1,2)-TS(IREC1).LE.EF(LABEL(IREC1,2))) GO TO 252
249   IREC1 = IREC1+1
      GOTO 248
  251 ENOR=ER(IREC1,2)*CXR(IREC1)*CXR(IREC1)
      IF(ENOR.GT.SBE(LABEL(IREC1,2))) GO TO 254
C
C     BACKREFLECTED RECOIL
C
      XR(IREC1,2)=-SU
      CSXR(IREC1,2)=-CSXR(IREC1,2)
      GO TO 248
C
C     SPUTTERED RECOIL
C
  254 ESP=ER(IREC1,2)-SBE(LABEL(IREC1,2))
C
```

```
C     TOTAL NUMBER AND ENERGY OF SPUTTERED PARTICLES
C
      IBSP(LABEL(IREC1,2))=IBSP(LABEL(IREC1,2))+1
      EBSP(LABEL(IREC1,2))=EBSP(LABEL(IREC1,2))+ESP
C
C     4 GROUPS:ION IN , PKA ;ION IN , SKA ;ION OUT, PKA ;ION OUT, SKA
C
      KOI=KO(IREC1,LABEL(IREC1,2),2)
      IF(INOUT(IREC1,2).EQ.-1) GO TO 61
      IF(KOI.EQ.0) GO TO 62
      ISPINP(LABEL(IREC1,2))=ISPINP(LABEL(IREC1,2))+1
      ESPINP(LABEL(IREC1,2))=ESPINP(LABEL(IREC1,2))+ESP
      GO TO 250
   62 ISPINS(LABEL(IREC1,2))=ISPINS(LABEL(IREC1,2))+1
      ESPINS(LABEL(IREC1,2))=ESPINS(LABEL(IREC1,2))+ESP
      GO TO 250
   61 IF(KOI.EQ.0) GO TO 163
      ISPOP(LABEL(IREC1,2))=ISPOP(LABEL(IREC1,2))+1
      ESPOP(LABEL(IREC1,2))=ESPOP(LABEL(IREC1,2))+ESP
      GO TO 250
  163 ISPOS(LABEL(IREC1,2))=ISPOS(LABEL(IREC1,2))+1
      ESPOS(LABEL(IREC1,2))=ESPOS(LABEL(IREC1,2))+ESP
      GOTO 250
C
C     RECOIL EXCEEDING TT
C
255   DEL(IXRV(IREC1),LABEL(IREC1,2))=DEL(IXRV(IREC1),LABEL(IREC1,2))+1.
      GOTO 250
C
C     RECOIL SLOWED DOWN
C
252   IXRC = IXRV(IREC1)
      IF(EORC(IREC1,2).GT.ED(LABEL(IREC1,2)).OR.IRCO.LT.0) GOTO 257
      IXRC = IXST(IREC1,2)
257   DEL(IXRC,LABEL(IREC1,2)) = DEL(IXRC,LABEL(IREC1,2))+1.
C
C     REARRANGEMENT OF PARTICLES IN LIST 2
C
250   IF(IREC1.GE.NREC2) GOTO 258
      ER(IREC1,2)=ER(NREC2,2)
      TS(IREC1)=TS(NREC2)
      XR(IREC1,2)=XR(NREC2,2)
      YR(IREC1,2)=YR(NREC2,2)
      ZR(IREC1,2)=ZR(NREC2,2)
      CSXR(IREC1,2)=CSXR(NREC2,2)
      CSYR(IREC1,2)=CSYR(NREC2,2)
      CSZR(IREC1,2)=CSZR(NREC2,2)
      SNXR(IREC1,2)=SNXR(NREC2,2)
```

```
      PHIR(IREC1,2)=PHIR(NREC2,2)
      PSIR(IREC1,2)=PSIR(NREC2,2)
      L(IREC1,2)=L(NREC2,2)
      LABEL(IREC1,2)=LABEL(NREC2,2)
      IXST(IREC1,2)=IXST(NREC2,2)
      EORC(IREC1,2)=EORC(NREC2,2)
      LMV(IREC1,2)=LMV(NREC2,2)
      KO(IREC1,LABEL(IREC1,2),2)=KO(NREC2,LABEL(NREC2,2),2)
      INOUT(IREC1,2)=INOUT(NREC2,2)
      IXRV(IREC1) = IXRV(NREC2)
      TEST(IREC1) = TEST(NREC2)
258   NREC2=NREC2-1
      IF(NREC2+1.GT.IVMAX) GO TO 249
      GOTO 248
C
C     ELASTIC ENERGY LOSS
C
  247 DO 256 IREC1=1,NREC2
      ER(IREC1,2)=ER(IREC1,2)-TS(IREC1)
  256 CONTINUE
C
C     END OF RECOIL ATOM SECTION
C
      IF(NREC1+NREC2.GT.MAXMAX) GOTO 75
      IF(NREC1+NREC2.GT.0) GOTO 73
C
C     DYNAMIC RELAXATION SECTION
C
      IF(IDREL.NE.0) GOTO 10
C
C     NEW AREAL DENSITIES
C
      DO 4180 JP=1,NCP
      DO 4180 MM=1,NQX
4180  DEL(MM,JP) = DEL(MM,JP)*FLC/NH
      DO 4182 MM=1,NQX
      DXV(MM) = XNO(MM+1)-XNO(MM)
      DNSOV(MM) = DNS(MM)
4182  SUMV(MM) = 0.
      DO 4184 JP=1,NCP
      DO 4184 MM=1,NQX
4184  SUMV(MM) = SUMV(MM)+DEL(MM,JP)
      DO 4186 MM=1,NQX
4186  CHAV(MM) = ABS(SUMV(MM))/DNSOV(MM)/DXV(MM)
      MM = ISMAX(NQX,CHAV,1)
      IF(CHAV(MM).GT.CHAMAX) CHAMAX = CHAV(MM)
      DO 4190 JP=1,NCP
      DO 4190 MM=1,NQX
```

```
4190  DEL(MM,JP) = DEL(MM,JP)+QUX(MM,JP)*DNSOV(MM)*DXV(MM)
C
C     PROJECTILE REEMISSION
C
      IF(QU1MX.GE.1.) GOTO 2350
      DO 4192 MM=1,NQX
4192  SUMV(MM) = 0.
      DO 4200 JP=2,NCP
      DO 4200 MM=1,NQX
4200  SUMV(MM) = SUMV(MM)+DEL(MM,JP)
      DO 4202 MM=1,NQX
      D1MXV(MM) = QU1MX*SUMV(MM)/(1.-QU1MX)
4202  TEST(MM) = DEL(MM,1).LE.D1MXV(MM)
      DO 4204 MM=1,NQX
      IF(TEST(MM)) GOTO 4204
      REEM1 = REEM1+DEL(MM,1)-D1MXV(MM)
      DEL(MM,1) = D1MXV(MM)
4204  CONTINUE
C
C     RELAXATION TO NEW INTERVAL THICKNESSES
C
2350  DO 2352 MM=1,NQX
2352  XXX(MM) = 0.
      DO 4210 JP=1,NCP
      DO 4210 MM=1,NQX
      XXX(MM) = XXX(MM)+DEL(MM,JP)/DNSO(JP)
4210  TEST(MM) = XXX(MM).LE.0.
      MM = ILSUM(NQX,TEST,1)
      IF(MM.LE.0) GOTO 2050
      WRITE(IO,2105)IH,MM,XXX(MM),NCPM,(DEL(MM,JP),JP=1,NCPM)
2105  FORMAT(5X,'IH=',I5,5X,'MM=',I5,5X,'XXX=',E12.4/
     C17X,'DEL1..',I1,'=',4(E12.4,1H,),E12.4/
     C5X,'DEPTH INTERVAL COMPLETELY DEPLETED'/
     C5X,'----- DECREASE FLC OR INCREASE NH -----')
      STOP
2050  SUMM = 0.
      DO 2052 MM=1,NQX
2052  SUMM = SUMM+XXX(MM)
C
C     SURFACE RECESSION
C
      DSRRC = XNO(NQX+1)-SUMM
      SRRCN = SRRCN+DSRRC
      SRRC = SRRC+DSRRC
C
C     COMBINATION OF TOO SMALL INTERVALS
C     SPLITTING OF TOO LARGE INTERVALS
C
```

```
      DO 4560 MM=1,NQX-2
4560  TEST(MM) = XXX(MM).LT..5*DQX.OR.XXX(MM).GT.1.5*DQX
      MM = ILSUM(NQX-2,TEST,1)
      IF(MM.LE.0) GOTO 4620
      DO 4562 MM=1,NQX-2
      IF(XXX(MM).GE..5*DQX) GOTO 4570
      XXX(MM) = XXX(MM)+XXX(MM+1)
      DO 4580 JP=1,NCP
4580  DEL(MM,JP) = DEL(MM,JP)+DEL(MM+1,JP)
      DO 4590 MMM=MM+1,NQX-1
4590  XXX(MMM) = XXX(MMM+1)
      DO 4600 JP=1,NCP
      DO 4600 MMM=MM+1,NQX-1
4600  DEL(MMM,JP) = DEL(MMM+1,JP)
      XXX(NQX) = DQX
      DO 4610 JP=1,NCP
4610  DEL(NQX,JP) = QUXB(JP)
4570  IF(XXX(MM).LE.1.5*DQX) GOTO 4562
      DO 4630 MMM=NQX-1,MM+1,-1
4630  XXX(MMM+1) = XXX(MMM)
      DO 4640 JP=1,NCP
      DO 4640 MMM=NQX-1,MM+1,-1
4640  DEL(MMM+1,JP) = DEL(MMM,JP)
      XXX(MM) = XXX(MM)/2.
      XXX(MM+1) = XXX(MM)
      DO 4650 JP=1,NCP
      DEL(MM,JP) = DEL(MM,JP)/2.
4650  DEL(MM+1,JP) = DEL(MM,JP)
4562  CONTINUE
C
C     ATOMIC FRACTIONS AND DENSITIES
C
4620  DO 4622 MM=1,NQX
      XNO(MM+1) = XNO(MM)+XXX(MM)
      DNS(MM) = 0.
4622  SUMV(MM) = 0.
      DO 4660 JP=1,NCP
      DO 4660 MM=1,NQX
4660  SUMV(MM) = SUMV(MM)+DEL(MM,JP)
      DO 4670 JP=1,NCP
      DO 4670 MM=1,NQX
      QUX(MM,JP) = DEL(MM,JP)/SUMV(MM)
4670  DNS(MM) = DNS(MM)+QUX(MM,JP)/DNSO(JP)
      DO 4672 MM=1,NQX
4672  DNS(MM) = 1./DNS(MM)
C
C     PROJECTILE REMOVAL AND READJUSTMENT OF DEPOSITION FUNCTIONS
C     DUE TO SURFACE RECESSION
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C
      IF(SRRCN.LT.DQX/2.) GOTO 2270
      J = (INT(2.*SRRCN/DQX)-1)/2+1
      SRRCN = SRRCN-J*DQX
      DO 2280 I=1,J
2280  IPREC = IPREC+IRP(I)
      DO 2290 I=1,NQX-J
      FPKP(I) = FPKP(I+J)
      IRP(I) = IRP(I+J)
      ION(I) = ION(I+J)
      NCLR(I) = NCLR(I+J)
      DMGN(I) = DMGN(I+J)
2290  PHON(I) = PHON(I+J)
      DO 2300 I=NQX-J+1,NQX
      FPKP(I) = 0.
      IRP(I) = 0
      ION(I) = 0.
      NCLR(I) = 0.
      DMGN(I) = 0.
2300  PHON(I) = 0.
C
C     CALCULATION AND OUTPUT OF INTEGRAL QUANTITIES
C
2270  IF(IDOUT.LE.0) GOTO 10
      IF(MOD(IH,IDOUT).NE.0) GOTO 10
      AMM = 0
      DO 4300 JP=1,NCP
      ARD(JP) = 0.
4300  CSF(JP) = 0.
      DO 4310 MM=1,NQX
      SUM = 0.
      DO 4320 JP=2,NCP
4320  SUM = SUM+QUX(MM,JP)
      DO 4330 JP=1,NCP
4330  ARD(JP) = ARD(JP)+QUX(MM,JP)*XXX(MM)*DNS(MM)
      IF(XNO(MM).GE.DSF) GOTO 4310
      DAM = 1.
      IF(XNO(MM+1).LE.DSF) GOTO 4720
      DAM = (DSF-XNO(MM))/XXX(MM)
4720  AMM = AMM+DAM
      DO 4340 JP=2,NCP
4340  CSF(JP) = CSF(JP)+QUX(MM,JP)/SUM*DAM
4310  CONTINUE
      IF(AMM.LE.0) GOTO 4350
      DO 4360 JP=2,NCP
4360  CSF(JP) = CSF(JP)/AMM
4350  DO 5000 JP=1,5
5000  FLIB(JP) = 0.
```

```
      IF(IMCP.LE.0) GOTO 4990
      DO 5010 MM=1,NQX
      SUM = XNO(MM)+XXX(MM)/2.
      FLIB(1) = FLIB(1)+QUX(MM,IMCP)*XXX(MM)*DNS(MM)
5010  FLIB(2) = FLIB(2)+QUX(MM,IMCP)*XXX(MM)*SUM*DNS(MM)
      IF(FLIB(1).LE.0.) GOTO 4990
      FLIB(2) = FLIB(2)/FLIB(1)
      DO 5020 MM=1,NQX
      SUM = XNO(MM)+XXX(MM)/2.
      SUMM = QUX(MM,IMCP)*XXX(MM)*DNS(MM)*(SUM-FLIB(2))**2
      FLIB(3) = FLIB(3)+SUMM
      FLIB(4) = FLIB(4)+SUMM*(SUM-FLIB(2))
5020  FLIB(5) = FLIB(5)+SUMM*(SUM-FLIB(2))**2
      IF(FLIB(3).LE.1.E-10*FLIB(2)) GOTO 5040
      FLIB(3) = SQRT(FLIB(3)/FLIB(1))
      FLIB(4) = FLIB(4)/FLIB(3)**3
      FLIB(5) = FLIB(5)/FLIB(3)**4-3.
      GOTO 4990
5040  FLIB(3) = 0.
      FLIB(4) = 0.
      FLIB(5) = 0.
4990  FLUC = FLC*IH/NH
      DO 4370 JP=1,NCP
      SPYD(JP) = (IBSP(JP)-IBSPO(JP))/FLOAT(IDOUT)
4370  IBSPO(JP) = IBSP(JP)
      WRITE(IO1,2035)FLUC,SRRC,REEM1,(CSF(JP),JP=2,NCPM),FLIB,SPYD,ARD
C
C     INTERPOLATION TO EQUIDISTANT INTERVALS AND OUTPUT OF PROFILES
C
      IF(IQOUT.LE.0) GOTO 10
      IF(MOD(IH,IQOUT).NE.0) GOTO 10
      DO 2340 MM=IQXN,IQXX
      XX0 = (MM-1)*DQX
      XX1 = MM*DQX
      DO 4220 JP=1,NCP
4220  SSUM(JP) = 0.
      XXX0 = 0.
      DO 2160 MMM=1,NQX
      XXX0 = XXX0+XXX(MMM)
2160  IF(XXX0.GT.XX0) GOTO 2170
      DO 4240 JP=1,NCP
4240  SSUM(JP) = QUXB(JP)*DQX*DNSB
      GOTO 2090
2170  DO 4250 JP=1,NCP
4250  SSUM(JP) = SSUM(JP)+(XXX0-XX0)/XXX(MMM)*DEL(MMM,JP)
      IF(XXX0-XX1)2180,2090,2200
2180  MMM = MMM+1
      IF(MMM.LE.NQX) GOTO 2210
```

```
      DO 4260 JP=1,NCP
4260  SSUM(JP) = SSUM(JP)+(XX1-XXX0)*QUXB(JP)*DNSB
      GOTO 2090
2210  XX0 = XXX0
      XXX0 = XXX0+XXX(MMM)
      GOTO 2170
2200  DO 4270 JP=1,NCP
4270  SSUM(JP) = SSUM(JP)-(XXX0-XX1)/XXX(MMM)*DEL(MMM,JP)
2090  SUM = 0.
      DO 4280 JP=1,NCP
4280  SUM = SUM+SSUM(JP)
      DNSI = 0.
      DO 4290 JP=1,NCP
      QUXI(JP) = SSUM(JP)/SUM
4290  DNSI = DNSI+QUXI(JP)/DNSO(JP)
      DNSI = 1./DNSI
      XXXI = (MM-.5)*DQX
2340  WRITE(IO1,2045)XXXI,DNSI,(QUXI(JP),JP=1,NCP)
C
C     END OF DYNAMIC RELAXATION SECTION
C
      GOTO 10
C
C     PRINTED OUTPUT
C
18    WRITE(IO,4055)AVSO,TITLE
4055  FORMAT(' DYNAMIC COMPOSITION TRIM PROGRAM     TRIDYN',
     C'      VERSION ',A3//1X,16A4//6X,
     C'NH   NCP  IDOUT IQOUT IDREL IQ0 IRCO IRAND JSP1 JSP2 JFRP JNRM')
      WRITE(IO,4065)NH,NCP,IDOUT,IQOUT,IDREL,IQ0,IRCO,IRAND,JSP1I,JSP2,
     CJFRP,JNRM
4065  FORMAT(1X,I9,I3,I8,I6,I5,I5,I4,I7,I4,3I5)
      WRITE(IO,4075)
4075  FORMAT(/4X,'FLC',9X,'E0',8X,'X0',4X,'ALPHA INEL INELR',
     C' IWC IWCR',3X,'SHTH')
      WRITE(IO,4085)FLC,E0,X0,ALPHA,INEL,INELR,IWC,IWCR,SHTH
4085  FORMAT(2E11.4,F7.2,F8.2,I4,3I5,F9.2)
      WRITE(IO,4095)
4095  FORMAT(/5X,'TT',8X,'TTDYN   NQX    DSF   IQXN IQXX IMCP')
      WRITE(IO,4105)TT,TTDYN,NQX,DSF,IQXN,IQXX,IMCP
4105  FORMAT(2E11.4,I4,F8.2,1X,3I5)
      WRITE(IO,4115)
4115  FORMAT(/' CPT.     Z      M     SBE     BE     ED   ',
     C'  EF     DNSO      CK      Q')
      SUM = '(MAX'
      SUMM = '.)  '
      DO 4390 JP=1,NCP
      WRITE(IO,4125)JP,ZZ(JP),M(JP),SBE(JP),BE(JP),ED(JP),EF(JP),
```

```
     CDNSO(JP),CK(JP),QUINP(JP),SUM,SUMM
4125  FORMAT(1X,I2,F8.0,F7.2,4F6.2,E11.4,F5.2,F6.3,2A4)
      IF(JP.GT.1) GOTO 4390
      IF(IQ0.NE.0) GOTO 4400
      SUM = '(INI'
      SUMM = 'T.) '
      GOTO 4390
4400  SUM = '(VAR'
      SUMM = 'BL.)'
4390  CONTINUE
      IF(IQ0.EQ.0) GOTO 5070
      WRITE(IO,4925)
4925  FORMAT(///' VARIABLE INITIAL COMPOSITION:')
      DO 5080 JP=2,NCP
5080  WRITE(IO,4935)JP,(QUX0(MM,JP),MM=1,NQX)
4935  FORMAT(/'  COMPONENT #',I1,':'/25(1X,20F6.3/))
5070  WRITE(IO,4135)
4135  FORMAT(///'  I',5X,'EPS0  A(I,J) KL(I,J) KOR(I,J) EC(I,J)'
     C,'   F(I,J)')
      DO 4410 JP=1,NCP
      WRITE(IO,4145)JP,EPS0(JP),A(JP,1),KL(JP,1),KOR(JP,1),EC(JP,1),
     CF(JP,1)
4145  FORMAT(1X,I2,F10.4,F7.4,2F8.4,F9.4,E11.4)
      DO 4410 MM=2,NCP
4410  WRITE(IO,4155)A(JP,MM),KL(JP,MM),KOR(JP,MM),EC(JP,MM),F(JP,MM)
4155  FORMAT(12X,3F8.4,F9.4,E11.4)
      WRITE(IO,483)MAXA,NALL,CHAMAX
483   FORMAT(//6X,'SIMREC =',I4,5X,'TOTREC =',I9,5X,'MAXCHA = ',F5.3)
      IF(IDREL.GE.0) WRITE(IO,2135)SRRC
2135  FORMAT(//6X,'FINAL SURFACE RECESSION =',F8.3,' A')
      IF(QU1MX.LT.1.) WRITE(IO,2145)REEM1
2145  FORMAT(/6X,'REEMITTED PROJECTILES   =',F8.3,' A-2')
      WRITE(IO,500)IB,EB,IT,ET,IPREC
  500 FORMAT(//6X,26HBACKSCATTERED PROJECTILES=,I8,5X,7HENERGY=,E10.4,
     1 3H EV/8X,24HTRANSMITTED PROJECTILES=,I8,5X,7HENERGY=,E10.4,3H EV/
     512X,20HREMOVED PROJECTILES=,I8)
      IBSPA = 0.
      EBSPA = 0.
      DO 4420 JP = 1,NCP
      IBSPA = IBSPA+IBSP(JP)
      EBSPA = EBSPA+EBSP(JP)
4420  WRITE(IO,4165)JP,IBSP(JP),EBSP(JP)
4165  FORMAT(9X,'SPUTTERED PARTICLES(',I1,')=',I8,5X,
     C'ENERGY=',E10.4,' EV')
      WRITE(IO,4175)IBSPA,EBSPA
4175  FORMAT(8X,24HALL SPUTTERED PARTICLES=,I8,5X,7HENERGY=,E10.4,3H EV)
       ISPINPA = 0
      ESPINPA = 0.
```

```
      ISPINSA = 0
      ESPINSA = 0.
      ISPOPA = 0
      ESPOPA = 0.
      ISPOSA = 0
      ESPOSA = 0.
      DO 4430 JP=1,NCP
      ISPINPA = ISPINPA+ISPINP(JP)
      ESPINPA = ESPINPA+ESPINP(JP)
      ISPINSA = ISPINSA+ISPINS(JP)
      ESPINSA= ESPINSA+ESPINS(JP)
      ISPOPA = ISPOPA+ISPOP(JP)
      ESPOPA = ESPOPA+ESPOP(JP)
      ISPOSA = ISPOSA+ISPOS(JP)
      ESPOSA = ESPOSA+ESPOS(JP)
4430  WRITE(IO,4185)JP,ISPINP(JP),ESPINP(JP),JP,ISPINS(JP),ESPINS(JP),
     CJP,ISPOP(JP),ESPOP(JP),JP,ISPOS(JP),ESPOS(JP)
4185  FORMAT(/5X,'     ION IN , PRIMARY KO(',I1,')=',I8,5X,'ENERGY=',
     CE10.4,' EV'/9X,'ION IN , SECOND. KO(',I1,')=',I8,5X,'ENERGY=',
     CE10.4,' EV'/9X,'ION OUT, PRIMARY KO(',I1,')=',I8,5X,'ENERGY=',
     CE10.4,' EV'/9X,'ION OUT, SECOND. KO(',I1,')=',I8,5X,'ENERGY=',
     CE10.4,' EV')
       WRITE(IO,1320)ISPINPA,ESPINPA,ISPINSA,ESPINSA,ISPOPA,ESPOPA,ISPOS
     1 A,ESPOSA
 1320  FORMAT(/3X,29H     ION IN , PRIMARY KO(ALL)=,I8,5X,7HENERGY=,E10.4
     1 ,3H EV/7X,25HION IN , SECOND. KO(ALL)=,I8,5X7HENERGY=,E10.4,3H EV
     2 /6X,26HION OUT , PRIMARY KO(ALL)=,I8,5X,7HENERGY=,E10.4,3H EV/
     3 6X,26HION OUT , SECOND. KO(ALL)=,I8,5X,7HENERGY=,E10.4,3H EV)
C
C     RANGE AND PATHLENGTH PARAMETERS
C
      YH=NH-IB-IT
      IF(YH.LE.0.) GOTO 12
      AVEX = XSUM/YH
      VARI = X2SUM/YH-AVEX**2
      SIGMAX= SQRT(VARI)
      AVEPL=PLSUM/YH
      AVECOL=FLOAT(ICSUM)/YH
      AVCOL=FLOAT(ICSUM1)/YH
      SIGMPL= SQRT(PL2SUM/YH-AVEPL**2)
      IF(SIGMAX.EQ.0.) GOTO 12
      U=AVEX/SIGMAX
      U2=U**2
      GAMMA = X3SUM/YH/SIGMAX**3-U*(3.+U2)
      BETA = X4SUM/YH/VARI**2-4.*U*GAMMA-U2*(6.+U2)
   12 WRITE(IO,800)AVEX,AVEPL,AVECOL,SIGMAX,SIGMPL,AVCOL,GAMMA,BETA
  800 FORMAT(//5X'  AVERAGE  DEPTH  ='F8.2,5X'AVERAGE PATHLENGTH='F8.2,
     15X'AVER. NUMBER COLL.='F8.1/5X'STANDARD DEVIATION='F8.2,5X'STANDAR
```

```
     2D DEVIATION='F8.2,5X'AV. NR. COLL.(ED) ='F8.1/5X,'  SKEWNESS GAMMA
     3  ='F8.2/5X'   KURTOSIS BETA  ='F8.2)
C
C     REFLECTION COEFFICIENTS AND SPUTTERING YIELDS
C
       EMEAN = 0.0
       RN = FLOAT(IB)/FLOAT(NH)
       RE = EB/NH/ABS(E0)
       WRITE(IO,810) RN,RE
  810 FORMAT(//5X,'REFL.COEFF.=',F8.5,'   ENERGY REFL.COEFF.=',F8.5)
      SPY=FLOAT(IBSPA)/FLOAT(NH)
      SPE=EBSPA/NH/ABS(E0)
      WRITE(IO,830) SPY,SPE
  830 FORMAT(/5X,'SPUTTERING YIELD(ALL) = ',1PE9.3,
     C'  SPUTTERED ENERGY(ALL) = ',E9.3)
      WRITE(IO,834)FPKTOT
834   FORMAT(/5X,'FRENKEL PAIRS (K/P) =',E11.4)
      WRITE(IO,833)(I,BBRTOT(I),I=1,NCP)
833   FORMAT(5X,'FRENKEL PAIRS (',I1,')   =',E11.4)
      WRITE(IO,832)IONTOT,NCLTOT,DMGTOT,PHOTOT
832   FORMAT(/8X,'INELASTIC ENERGY LOSS =',E11.4,' EV',
     C10X,'ELASTIC ENERGY LOSS =',E11.4,' EV'/6X,'ENERGY LOSS INTO',
     C' DAMAGE =',E11.4,' EV',5X,'ENERGY LOSS INTO PHONONS =',E11.4,
     C' EV'/)
C
C     DEPOSITION PROFILES
C
485   FORMAT(/////10X,'PSEUDOPROJECTILE DEPOSITION PROFILES:')
      WRITE(IO,600)
  600 FORMAT(///4X,8HDEPTH(A),2X,9HPARTICLES,1X,6HPATHL.,
     12X,15HFRENKEL P.(K/P),2X,10HELECTR(EV),4X,11HNUCLEAR(EV),5X,
     C10HDAMAGE(EV),4X,11HPHONONS(EV)/)
      D1=0.
      D2=DQX
      DO 19 MM=NQX,1,-1
19    IF(IPL(MM).NE.0) GOTO 20
      MM = 1
20    MM = MM+2
      DO 11 I=1,MM
      WRITE(IO,700) D1,D2,IRP(I),IPL(I),FPKP(I),ION(I),NCLR(I),DMGN(I),
     CPHON(I)
  700 FORMAT(1X,F6.0,1H-,F5.0,2I8,5E15.4)
      D1=D2
   11 D2=D2+DQX
C
C     INTERPOLATION AND OUTPUT OF DEPOSITION PROFILES
C
      DO 4470 MM=1,NQX
```

```
      IF(IDREL.NE.0) GOTO 4472
      XX0 = (MM-1)*DQX
      XX1 = MM*DQX
      DO 4222 JP=1,NCP
 4222 SSUM(JP) = 0.
      XXX0 = 0.
      DO 2162 MMM=1,NQX
      XXX0 = XXX0+XXX(MMM)
 2162 IF(XXX0.GT.XX0) GOTO 2172
      DO 4242 JP=1,NCP
 4242 SSUM(JP) = QUXB(JP)*DQX*DNSB
      GOTO 2092
 2172 DO 4252 JP=1,NCP
 4252 SSUM(JP) = SSUM(JP)+(XXX0-XX0)/XXX(MMM)*DEL(MMM,JP)
      IF(XXX0-XX1)2182,2092,2202
 2182 MMM = MMM+1
      IF(MMM.LE.NQX) GOTO 2212
      DO 4262 JP=1,NCP
 4262 SSUM(JP) = SSUM(JP)+(XX1-XXX0)*QUXB(JP)*DNSB
      GOTO 2092
 2212 XX0 = XXX0
      XXX0 = XXX0+XXX(MMM)
      GOTO 2172
 2202 DO 4272 JP=1,NCP
 4272 SSUM(JP) = SSUM(JP)-(XXX0-XX1)/XXX(MMM)*DEL(MMM,JP)
 2092 SUM = 0.
      DO 4282 JP=1,NCP
 4282 SUM = SUM+SSUM(JP)
      DO 4292 JP=1,NCP
 4292 QUX(MM,JP) = SSUM(JP)/SUM
 4472 DNS(MM) = 0.
      SUM = 0.
      DO 4294 JP=JNRM,NCP
      DNS(MM) = DNS(MM)+QUX(MM,JP)/DNS0(JP)
 4294 SUM = SUM+QUX(MM,JP)
      DNS(MM) = SUM/DNS(MM)
 4470 FACT(MM) = FLC/NH/DNS(MM)/DQX
      DO 4770 MM=1,NQX
      RION(MM) = IRP(MM)
 4770 XXX(MM) = (MM-.5)*DQX*1.E-8
      WRITE(IO2,4775)TITLE
 4775 FORMAT(' Range Distrib. ',16A4)
      CALL TRUNC(RION,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),RION(MM),MM=1,N)
      DO 4780 MM=1,NQX
 4780 RION(MM) = IPL(MM)
      WRITE(IO2,4785)TITLE
 4785 FORMAT(' Pathlength D.  ',16A4)
```

```
      CALL TRUNC(RION,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),RION(MM),MM=1,N)
      WRITE(IO2,4795)TITLE
4795  FORMAT(' Frenkel P.(K/P)',16A4)
      CALL TRUNC(FPKP,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),FPKP(MM),MM=1,N)
      WRITE(IO2,4805)TITLE
4805  FORMAT(' Electr. Losses ',16A4)
      CALL TRUNC(ION,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),ION(MM),MM=1,N)
      WRITE(IO2,4815)TITLE
4815  FORMAT(' Nuclear Losses ',16A4)
      CALL TRUNC(NCLR,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),NCLR(MM),MM=1,N)
      WRITE(IO2,4825)TITLE
4825  FORMAT(' Damage Losses  ',16A4)
      CALL TRUNC(DMGN,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),DMGN(MM),MM=1,N)
      WRITE(IO2,4835)TITLE
4835  FORMAT(' Phonon Losses  ',16A4)
      CALL TRUNC(PHON,FACT,NQX,N)
      WRITE(IO2,4205)(XXX(MM),PHON(MM),MM=1,N)
      DO 4830 JP=1,NCP
      WRITE(IO2,4845)JP,TITLE
4845  FORMAT(' Cpt',I1,' Frenkel P.',16A4)
      CALL TRUNC(BBR(1,JP),FACT,NQX,N)
4830  WRITE(IO2,4205)(XXX(MM),BBR(MM,JP),MM=1,N)
4205  FORMAT(2E15.6)
      STOP
      END
C
C
C
      SUBROUTINE TRUNC(A,B,NO,N)
      DIMENSION A(1),B(1)
      DO 10 I=NO,3,-1
10    IF(A(I).NE.0.) GOTO 20
      I = 3
20    N = MIN0(I+2,NO)
      DO 30 I=1,N
30    A(I) = A(I)*B(I)
      RETURN
      END
C
C
C
      SUBROUTINE DIRCOS(COSX,COSY,COSZ,SINE,PSI,PHI)
      CPHI=COS(PHI)
```

```
      SPHI=SIN(PHI)
      CPSI=COS(PSI)
      SPSI=SIN(PSI)
      SRAT=SPSI/SINE
      CX2=CPSI*COSX+SPSI*SINE*CPHI
      CY2=CPSI*COSY-SRAT*(COSY*COSX*CPHI-COSZ*SPHI)
      CZ2=CPSI*COSZ-SRAT*(COSZ*COSX*CPHI+COSY*SPHI)
      UNIT = 1.0/SQRT(CX2**2+CY2**2+CZ2**2)
      COSX=CX2*UNIT
      COSY=CY2*UNIT
      COSZ=SIGN(ABS(CZ2*UNIT)+1.E-12,CZ2)
      SINE=SQRT(COSY*COSY+COSZ*COSZ)
      RETURN
      END
C
C
C
      SUBROUTINE DIRCOSV(COSX,COSY,COSZ,SINE,PSI,PHI,N)
      DIMENSION PHI(N),PSI(N),COSX(N),COSY(N),COSZ(N),SINE(N)
      DO 1 IV=1,N
      CPHI=COS(PHI(IV))
      SPHI=SIN(PHI(IV))
      CPSI=COS(PSI(IV))
      SPSI=SIN(PSI(IV))
      SRAT=SPSI/SINE(IV)
      CX2=CPSI*COSX(IV)+SPSI*SINE(IV)*CPHI
      CY2=CPSI*COSY(IV)-SRAT*(COSY(IV)*COSX(IV)*CPHI-COSZ(IV)*SPHI)
      CZ2=CPSI*COSZ(IV)-SRAT*(COSZ(IV)*COSX(IV)*CPHI+COSY(IV)*SPHI)
      UNIT = 1.0/SQRT(CX2**2+CY2**2+CZ2**2)
      COSX(IV)=CX2*UNIT
      COSY(IV)=CY2*UNIT
      COSZ(IV)=SIGN(ABS(CZ2*UNIT)+1.E-12,CZ2)
      SINE(IV)=SQRT(COSY(IV)*COSY(IV)+COSZ(IV)*COSZ(IV))
    1 CONTINUE
      RETURN
      END
C
C
C
      SUBROUTINE MXVELO(E,COSX,COSY,COSZ,SINE)
C
C     FETCH ENERGY AND VELOCITY FROM A MAXWELLIAN FLUX AT A SURFACE
C
      REAL M1
      COMMON/A/ M1,VELC,ZARG
      DATA PI2/6.283185/
C
      AR = ALOG(RANF())
```

```
      VELX=SQRT(-2.*AR)*ZARG
      ZZ = PI2*RANF()
      ZSIN = SIN(ZZ)
      ZCOS = COS(ZZ)
      AR = ALOG(RANF())
      ZT = SQRT(-2.*AR)
      VELY = ZT*ZCOS*ZARG
      VELZ = ZT*ZSIN*ZARG
      IF(VELC.GT.0.) VELX = SQRT(VELC+VELX**2)
      VELQ=VELX*VELX+VELY*VELY+VELZ*VELZ
      VEL=SQRT(VELQ)
      COSX=VELX/VEL
      COSY=VELY/VEL
      COSZ=VELZ/VEL
      COSZ = SIGN(ABS(COSZ)+1.E-12,COSZ)
      SINE=SQRT(COSY*COSY+COSZ*COSZ)
      E=M1*VELQ
      RETURN
      END
C
C
C
```

Appendix 2

Test Run Input

(Channel 5)

```
1 keV Ne->Ta2O5     60000 Hist. 6e16/cm2                                        1655
    60000 1200 6000     3     0     0    -1  2003     0     1     2     2       1656
  0.600E+1    1000.00      0.00        0.00     1     3     2     2             1657
  0.100E+5  0.200E+3   80  0.500E+1     0   100     1                           1658
  10.00   20.18    0.00    0.00    0.00    5.00   0.200   0.100E+0  1.00        1659
  73.00  180.95    8.10    0.00   50.00    8.00   0.286   0.554E-1  1.00        1660
   8.00   16.01    6.70    0.00   50.00    6.50   0.714   0.809E-1  1.00        1661
```

Appendix 3

Test Run Output

(Channel 6)

```
1 keV Ne->Ta2O5      60000 Hist. 6e16/cm2

     NH   NCP   IDOUT IQOUT IDREL IQ0 IRCO IRAND JSP1 JSP2 JFRP JNRM
   60000  3     1200  6000    0    0   -1   2003   0    0    2    2

   FLC          E0          X0     ALPHA INEL INELR IWC IWCR    SHTH
0.6000E+01 0.1000E+04   0.00     0.00    1    3    2    2      0.00

    TT         TTDYN   NQX     DSF    IQXN IQXX IMCP
0.1000E+05 0.2000E+03  80     5.00      1   80    1

CPT.     Z      M     SBE    BE    ED     EF     DNSO      CK     Q
 1      10.   20.18  0.00  0.00  0.00  5.00 0.1000E+00 1.00 0.200(MAX.)
 2      73.  180.95  8.10  0.00 50.00  8.00 0.5540E-01 1.00 0.286(INIT.)
 3       8.   16.01  6.70  0.00 50.00  6.50 0.8090E-01 1.00 0.714(INIT.)


 I     EPS0   A(I,J) KL(I,J) KOR(I,J) EC(I,J)    F(I,J)
 1    0.0475 0.1369  1.4001   0.9250   1.0000 0.4755E-04
             0.0908  2.7810   4.1753   0.3611 0.7774E-05
             0.1420  1.2471   0.7664   0.9867 0.5452E-04
 2    0.0078 0.0908  1.2935   1.9420   0.3611 0.8670E-06
             0.0706  4.7540  11.8188   1.0000 0.4600E-06
             0.0926  1.0815   1.5623   0.2987 0.8951E-06
 3    0.0545 0.1420  1.3490   0.8291   0.9867 0.6872E-04
             0.0926  2.5153   3.6334   0.2987 0.1012E-04
             0.1475  1.2116   0.6898   1.0000 0.8003E-04

     SIMREC =  35      TOTREC =  8390463      MAXCHA = 0.015

     FINAL SURFACE RECESSION =  33.726 A

     REEMITTED PROJECTILES    =   2.959 A-2

     BACKSCATTERED PROJECTILES=     9639      ENERGY=0.3720E+07 EV
       TRANSMITTED PROJECTILES=        0      ENERGY=0.0000E+00 EV
           REMOVED PROJECTILES=    17584
        SPUTTERED PARTICLES(1)=    12909      ENERGY=0.4959E+06 EV
        SPUTTERED PARTICLES(2)=     7310      ENERGY=0.1805E+06 EV
        SPUTTERED PARTICLES(3)=    22968      ENERGY=0.1186E+07 EV
       ALL SPUTTERED PARTICLES=    43187      ENERGY=0.1863E+07 EV

        ION IN , PRIMARY KO(1)=     2666      ENERGY=0.1735E+06 EV
        ION IN , SECOND. KO(1)=     5554      ENERGY=0.1073E+06 EV
        ION OUT, PRIMARY KO(1)=     2205      ENERGY=0.1668E+06 EV
        ION OUT, SECOND. KO(1)=     2484      ENERGY=0.4835E+05 EV

        ION IN , PRIMARY KO(2)=      537      ENERGY=0.1761E+05 EV
        ION IN , SECOND. KO(2)=     2584      ENERGY=0.3613E+05 EV
        ION OUT, PRIMARY KO(2)=     2153      ENERGY=0.8932E+05 EV
        ION OUT, SECOND. KO(2)=     2036      ENERGY=0.3739E+05 EV

        ION IN , PRIMARY KO(3)=     6367      ENERGY=0.4863E+06 EV
        ION IN , SECOND. KO(3)=     8203      ENERGY=0.1992E+06 EV
        ION OUT, PRIMARY KO(3)=     4866      ENERGY=0.4144E+06 EV
        ION OUT, SECOND. KO(3)=     3532      ENERGY=0.8656E+05 EV
```

```
  ION IN , PRIMARY KO(ALL)=    9570     ENERGY=0.6775E+06 EV
  ION IN , SECOND. KO(ALL)=   16341     ENERGY=0.3426E+06 EV
 ION OUT , PRIMARY KO(ALL)=    9224     ENERGY=0.6705E+06 EV
 ION OUT , SECOND. KO(ALL)=    8052     ENERGY=0.1723E+06 EV


  AVERAGE  DEPTH  =   26.26    AVERAGE PATHLENGTH=   54.08    AVER. NUMBER COLL.=    25.0
STANDARD DEVIATION=   14.27    STANDARD DEVIATION=   17.02    AV. NR. COLL.(ED) =    10.0
  SKEWNESS GAMMA  =    0.57
   KURTOSIS BETA  =    3.09

REFL.COEFF.= 0.16065   ENERGY REFL.COEFF.= 0.06200

SPUTTERING YIELD(ALL) = 7.198E-01  SPUTTERED ENERGY(ALL) = 3.105E-02

FRENKEL PAIRS (K/P) = 0.2416E+06
FRENKEL PAIRS (1)   = 0.1622E+07
FRENKEL PAIRS (2)   = 0.8877E+05
FRENKEL PAIRS (3)   = 0.2158E+06

  INELASTIC ENERGY LOSS = 0.8062E+07 EV          ELASTIC ENERGY LOSS = 0.4813E+08 EV
 ENERGY LOSS INTO DAMAGE = 0.3769E+08 EV     ENERGY LOSS INTO PHONONS = 0.1044E+08 EV
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DEPTH(A)	PARTICLES	PATHL.	FRENKEL P.(K/P)	ELECTR(EV)	NUCLEAR(EV)	DAMAGE(EV)	PHONONS(EV)
0.- 2.	2575	0	0.1417E+05	0.5137E+06	0.2839E+07	0.2246E+07	0.5934E+06
2.- 5.	2701	6	0.1353E+05	0.4648E+06	0.2742E+07	0.2166E+07	0.5756E+06
5.- 7.	2759	25	0.1199E+05	0.4083E+06	0.2477E+07	0.1933E+07	0.5437E+06
7.- 10.	2618	72	0.1082E+05	0.3541E+06	0.2227E+07	0.1730E+07	0.4962E+06
10.- 12.	2537	103	0.9510E+04	0.3018E+06	0.1981E+07	0.1523E+07	0.4583E+06
12.- 15.	2400	166	0.8362E+04	0.2543E+06	0.1744E+07	0.1330E+07	0.4142E+06
15.- 17.	2341	261	0.7292E+04	0.2110E+06	0.1529E+07	0.1155E+07	0.3739E+06
17.- 20.	2158	367	0.6320E+04	0.1718E+06	0.1313E+07	0.9814E+06	0.3312E+06
20.- 22.	1909	497	0.5281E+04	0.1383E+06	0.1102E+07	0.8161E+06	0.2861E+06
22.- 25.	1791	623	0.4494E+04	0.1099E+06	0.9320E+06	0.6875E+06	0.2445E+06
25.- 27.	1593	799	0.3646E+04	0.8700E+05	0.7749E+06	0.5627E+06	0.2122E+06
27.- 30.	1372	1008	0.2932E+04	0.6734E+05	0.6172E+06	0.4427E+06	0.1745E+06
30.- 32.	1202	1233	0.2260E+04	0.5292E+05	0.4860E+06	0.3406E+06	0.1454E+06
32.- 35.	1002	1503	0.1758E+04	0.4166E+05	0.3872E+06	0.2641E+06	0.1231E+06
35.- 37.	847	1730	0.1399E+04	0.3158E+05	0.3020E+06	0.2028E+06	0.9914E+05
37.- 40.	669	2013	0.1058E+04	0.2443E+05	0.2303E+06	0.1514E+06	0.7887E+05
40.- 42.	551	2276	0.7212E+03	0.1811E+05	0.1667E+06	0.1043E+06	0.6244E+05
42.- 45.	432	2562	0.6484E+03	0.1346E+05	0.1335E+06	0.8666E+05	0.4685E+05
45.- 47.	368	2653	0.4481E+03	0.1010E+05	0.9719E+05	0.5906E+05	0.3814E+05
47.- 50.	262	2829	0.3298E+03	0.7174E+04	0.6831E+05	0.4140E+05	0.2692E+05
50.- 52.	180	2841	0.2123E+03	0.5021E+04	0.4659E+05	0.2533E+05	0.2127E+05
52.- 55.	158	2911	0.1527E+03	0.3452E+04	0.3309E+05	0.1833E+05	0.1475E+05
55.- 57.	106	2930	0.1132E+03	0.2403E+04	0.2342E+05	0.1225E+05	0.1116E+05
57.- 60.	69	2847	0.8421E+02	0.1627E+04	0.1555E+05	0.7833E+04	0.7718E+04
60.- 62.	62	2673	0.4852E+02	0.1208E+04	0.1129E+05	0.5357E+04	0.5933E+04
62.- 65.	38	2516	0.2801E+02	0.6692E+03	0.6366E+04	0.2704E+04	0.3663E+04
65.- 67.	25	2226	0.1830E+02	0.4799E+03	0.3858E+04	0.1680E+04	0.2179E+04
67.- 70.	16	1961	0.9224E+01	0.3037E+03	0.2340E+04	0.8970E+03	0.1443E+04
70.- 72.	12	1747	0.1206E+02	0.2444E+03	0.2178E+04	0.9430E+03	0.1235E+04
72.- 75.	5	1437	0.2000E+01	0.1774E+03	0.1023E+04	0.1305E+03	0.8926E+03
75.- 77.	7	1196	0.3000E+01	0.9537E+02	0.7024E+03	0.2322E+03	0.4703E+03
77.- 80.	2	994	0.1000E+01	0.7566E+02	0.3595E+03	0.6211E+02	0.2974E+03
80.- 82.	1	826	0.2000E+01	0.5345E+02	0.4852E+03	0.1718E+03	0.3133E+03

82.- 85.	5	651	0.4118E+01	0.3697E+02	0.5537E+03	0.3647E+03	0.1890E+03
85.- 87.	2	479	0.0000E+00	0.3828E+02	0.3247E+03	0.0000E+00	0.3247E+03
87.- 90.	0	389	0.0000E+00	0.8001E+01	0.1613E+02	0.0000E+00	0.1613E+02
90.- 92.	0	291	0.0000E+00	0.9183E+01	0.5141E+02	0.0000E+00	0.5141E+02
92.- 95.	1	197	0.9025E+00	0.6527E+01	0.1515E+03	0.1289E+03	0.2253E+02
95.- 97.	1	149	0.0000E+00	0.7312E+01	0.9985E+02	0.0000E+00	0.9985E+02
97.- 100.	0	112	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
100.- 102.	0	84	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
102.- 105.	0	58	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
105.- 107.	0	37	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
107.- 110.	0	28	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
110.- 112.	0	18	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
112.- 115.	0	12	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
115.- 117.	0	10	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
117.- 120.	0	7	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
120.- 122.	0	5	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
122.- 125.	0	1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
125.- 127.	0	1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
127.- 130.	0	1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
130.- 132.	0	0	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
132.- 135.	0	0	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

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