MODIFICATIONS TO THE TRIM MONTE CARLO
SIMULATION PROGRAM

by

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MODIFICATIONS TO THE TRIM MONTE CARLO SIMULATION PROGRAM*

by

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ABSTRACT

Extensive modifications were made to the TRIM (Transport of Ions in Matter) Monte Carlo computer code (developed by J. Biersack and L. Haggmark) which simulates the ion irradiation of amorphous solids. The original FORTRAN code was translated into BASIC for use on minicomputers with 32K words of memory. Versions have been written to simulate very low-energy irradiations and the irradiation of binary alloys. Furthermore, a version was written which added the capability of following a lateral direction, in addition to the penetration depth of an ion. Subsequently, a version was written to simulate the production of collision cascades. Details of these modifications were discussed and examples of their use were given.

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1. INTRODUCTION

In 1978 the authors of the TRIM (Transport of Ions in Matter) Monte Carlo simulation code, J.P. Biersack and L.G. Haggmark, were kind enough to provide the research group headed by Professor D.N. Seidman at Cornell a copy of the FORTRAN listing of their program as part of an advanced preprint of an article describing it.⁽¹⁾ TRIM simulates ion irradiations of solids by following the history of a projectile through its successive collisions with atoms of the target, that is, in the binary collision approximation. An amorphous solid (no local or global periodicities) was assumed and, therefore, single crystal effects such as channeling were not incorporated. By following M (where M is large) histories, the program arrives at distributions for the total pathlength, projected range, electronic energy loss, nuclear energy loss, and damage (via the energy lost to recoil atoms). In addition, reflection coefficients are determined.

Of primary usefulness to the Cornell group was the ability to determine simulated mean ranges and range profiles to compare to experimental atom-probe field-ion microscope (APFIM) data.⁽²⁾ Due to the availability of a 32K word Nova 1220 minicomputer it appeared worthwhile to install the TRIM code at Cornell. For several reasons it was convenient to do so by translating from FORTRAN into BASIC. The BASIC interpreter is admittedly slow but because the single user minicomputer was dedicated to group use and because it could be run overnight to obtain a single result, this was not a great loss.

The original TRIM program, though quite general, was written to apply to considerably higher values of projectile energy than were of interest in APFIM experiments. The test of any computer simulation is, of course, its ability to predict experimental results, and the validity of TRIM was thus based on existing experimental data. Indeed, owing to the paucity of data at very low

energies, comparisons between APFIM results and TRIM simulations may be regarded as tests of the assumptions made and of the energy loss expressions used. For example, measured depth profiles deeper than predicted may be an indication that channeling along low-index directions is significant even at very low implantation energies. A BASIC language version of TRIM was written to apply specifically to very low energies. This was accomplished during two visits made by Dr. J.P. Biersack, of the Hahn-Meitner-Institute, to the Department of Materials Science and Engineering. The BASIC code eliminated those parts of the original TRIM that were no longer apropos and incorporated additional modifications believed to be important only at very low energies. This version of TRIM will be referred to as TRIM: LOW ENERGY.* Detailed comparisons of APFIM data for He on the (110) plane of tungsten, to TRIM: LOW ENERGY results have already been made.^(3,4) Furthermore, it was found useful in understanding APFIM data for H on the (110) plane of tungsten.⁽⁵⁾

Other workers under the direction of Professor Seidman subsequently found it useful to have versions of the program tailored to simulate their experiments. The readiness with which this can be done is presently considered a very powerful aspect of TRIM.

A version was written to apply to alloys and will be referred to as TRIM: ALLOY.* Detailed comparisons of field-ion microscope (FIM) data on Ni_4Mo and Pt_3Co with results obtained using this version have been made.^(4,6)

The original TRIM code kept track of only one dimension, the depth into the crystal. A code was written that kept track of a lateral dimension as well. This version will be referred to as TRIM: TRAJECTORY.* With this version the actual paths of the projectiles could be followed on line on a cathode ray tube display. Figures generated using this version have already been presented.⁽⁶⁾

From TRIM: TRAJECTORY it is an easy step to include a threshold energy for atomic displacements and to follow the recoiling atoms as well. Such a

*For a listing see the appendixes.

version has also been written and will be referred to as TRIM: CASCADE.*

Detailed comparisons between FIM experiments, in which the vacancy structure of depleted zones was analyzed with atomic resolution, and TRIM: CASCADE have also already been made.⁽⁵⁾ In addition, the original TRIM translated into BASIC, which will be referred to here as TRIM: BASIC, has proved useful in understanding FIM data on depleted zones.^(4,5,7,8)

It is the purpose of this report to document the various BASIC language versions of the TRIM code and to illustrate some of the computer results.

2. TRIM: LOW ENERGY

A. Low Energy Modifications

For high energies, defined as $\epsilon > 10$, the TRIM code chooses the distance between collisions, L , "such that the mean angular deflection per path length L remains constant."⁽¹⁾ The reduced energy (ϵ) is given by

$$\epsilon = a_F E_c / Z_1 Z_2 e^2 \quad (1)$$

In this relation a_F is the Firsov screening length⁽⁹⁾ given by

$$a_F = \frac{0.8853 a_0}{(Z_1^{1/2} + Z_2^{1/2})^{2/3}} \quad (2)$$

where $a_0 = 0.529 \text{ \AA}$ is the Bohr radius, Z_1 and Z_2 are the atomic numbers of the projectile and of the target, respectively, and E_c is the energy in the center-of-mass system given by

$$E_c = E (1 + M_1/M_2)^{-1}; \quad (3)$$

where E is the projectile energy and M_1 and M_2 are the atomic masses of the projectile and target atoms, respectively. At low energies L becomes less than the approximate mean interatomic separation given by

$$N_d^{-1/3} = (\rho N_a / M_2)^{-1/3} \quad (4)$$

where ρ is the density in gm cm^{-3} of the target and N_a is Avogadro's number.

TRIM then sets L equal to $N_d^{-1/3}$. For all the cases of interest to the

*For a listing see the appendixes.

Cornell group ϵ is less than 10. The test for high or low energy was, therefore, entirely removed. However, L was not set equal to $N_d^{-1/3}$. At very low energies the dimensions of the atoms must be included in calculating L . This was accomplished by shortening L by $P \tan(\theta/2)$ where P is the impact parameter and θ is the polar scattering angle in the center-of-mass system. This decrease in the pathlength is the hard-core value for the more general time integral, τ , of Robinson and Torrens.⁽¹⁰⁾

TRIM: LOW ENERGY uses exclusively an expression for the electronic energy loss due to Oen and Robinson,⁽¹¹⁾

$$\Delta E_e(E, r_o) = \frac{0.045 k \sqrt{E}}{\pi a_F^2} \exp(-0.3 r_o/a_F), \quad (5)$$

where k is the Linhard-Scharff⁽¹²⁾ velocity dependent stopping parameter, k_L , times a correction factor to include Z_1 or Z_2 oscillations,⁽¹³⁾ and r_o is the distance of closest approach.

A further modification involved the treatment of the arctangent function used to obtain the scattering angle in the laboratory system, ψ , given by

$$\tan \psi = \frac{\sin \theta}{(M_1/M_2) + \cos \theta} \quad (6)$$

In FORTRAN the statement $Y=ATAN(X)$ results in values of Y lying in the range $-\pi/2$ to zero for X less than zero and zero to $\pi/2$ for X greater than zero. Back-scattered events are thus not possible; negative values of X are treated erroneously in TRIM. At high energies this fact makes very little difference as fig. 1 shows. However, at low energies backscattered events are common as shown in fig. 2; the random walk nature of these trajectories requires a correct treatment of back-scattered events. TRIM: LOW ENERGY does this by adding π to the arctangent if $ATAN(X)$ is negative.

A final modification involved the angle of incidence. TRIM was set up to allow any angle desired. TRIM: LOW ENERGY, however allows only normal incidence.

The change is minor and a variable angle of incidence can easily be included.

B. Random Number Sequence

No discussion of a Monte Carlo program would be complete without a discussion of the random number sequence used. The NOVA 1220 is a 16 bit machine for which Data General supplied a (pseudo) random number sequence of $2^{16}-1=65,535$ random numbers. These are generated using the function: RND. The sequence is described as being linear and congruential.⁽¹⁴⁾ TRIM: LOW ENERGY requires two random numbers per collision-- one for the impact parameter and the other for the azimuthal (ϕ) scattering angle. To stretch the random number sequence the scheme in the Table was incorporated in TRIM: LOW ENERGY. In general, it proved possible to follow only about $M=1000$ histories. Typical examples of the number of ions remaining inside the solid with this scheme out of $M=1000$ projectile histories are: 340 (660 reflected) for 300 eV ^4He on W and 297 (703 reflected) for 100 eV ^1H on W. A larger and perhaps better random number sequence would improve matters considerably.

C. Illustration

To illustrate TRIM: LOW ENERGY the computer results for the case of 300 eV ^4He on W are shown in figs. 3 and 4. The histograms are not smooth. The extent to which they are not is due both to the small number of events--only 34% were implanted--and to the deficiencies of the random number generator.

In addition, the reflection coefficients--both the fraction of ions backscattered (R_N) and the fraction of the incident energy backscattered (R_E) for two ^4He on W runs and six ^1H on W runs are exhibited in fig. 5. These compare quite favorably to the results obtained using MARLOWE (a binary collision single crystal Monte Carlo simulation program) upon "rotating the target crystal randomly in three dimensions about a lattice site before each collision."⁽¹⁶⁾ Recently, a detailed comparison of TRIM and MARLOWE, has appeared in the literature. Particular emphasis was paid to reflection coefficients and quite good general agreement was found.⁽¹⁷⁾

3. TRIM: ALLOY

A version of TRIM was written to simulate irradiations of alloys of the form $A_{n-1}B$.⁽¹⁵⁾ For Pt_3Co , for example, the value $n=4$ must be supplied as part of the program input. The approximate mean interatomic spacing was chosen using

$$N_d^{-1/3} = \frac{\rho N_a}{\frac{n-1}{n} M_A + \frac{1}{n} M_B}^{-1/3} \quad (7)$$

where M_A and M_B are the atomic masses of elements A and B, respectively. In addition, the target atoms are chosen randomly to be of type A or B but with a frequency of $n-1$ to 1. This was achieved by evaluating the test

$$RND < n^{-1} \quad (8)$$

where RND is a random number. If true, an atom of type B was chosen as the target atom; alternatively, if false, an atom of type A was chosen.

4. TRIM: TRAJECTORY

The original TRIM employed the recursion relations

$$z_o^j = z_o^{j-1} + L_j \cos \alpha_j \quad (9)$$

$$\cos \alpha_j = \cos \alpha_{j-1} \cos \psi + \sin \alpha_{j-1} \sin \psi \cos \phi \quad (10)$$

to calculate the projected range of a single projectile in the solid.⁽¹⁾ Here z_o^j is the projected range after j collisions and α_j is the polar angle of the trajectory with respect to the surface normal after scattering. A Cartesian reference frame fixed in the solid, $(\hat{x}_o, \hat{y}_o, \hat{z}_o)$, in addition to the reference frame usually chosen for a collision, $(\hat{x}, \hat{y}, \hat{z})$, are shown in fig. 6. The x_o - y_o plane is chosen parallel to the surface, and the target atom is chosen to lie at the origin. Also $\hat{z}$ is chosen to be along the incident direction, $\hat{i}$, and $\hat{x}$ is chosen to lie in x_o - y_o plane. The coordinates of the unit vectors, $-\hat{i}$, $\hat{s}$, $\hat{x}$, $\hat{y}$ are also shown in fig. 6. In addition, three basic relations are given in fig. 6. Here ψ and ϕ are the usual polar and azimuthal scattering angles, that is, the polar and azimuthal angles of $\hat{s}$ in the $(\hat{x}, \hat{y}, \hat{z})$ frame.

It is clear that

$$\begin{aligned}\alpha_j &= \theta_s \\ \alpha_{j-1} &= \pi - \theta_i\end{aligned}\quad (11)$$

To plot a trajectory, however, one needs as well a recursion relation for β_j where

$$\begin{aligned}\beta_j &= \phi_s \\ \beta_{j-1} &= \pi + \phi_i\end{aligned}\quad (12)$$

which can then be used in

$$x_o^j = x_o^{j-1} + L_j \sin \alpha_j \cos \beta_j \quad (13)$$

to keep track of the lateral motion of the project. Here the $\hat{x}_o$ direction is chosen, but having done this, y_o^j is just as easily followed via

$$y_o^j = y_o^{j-1} + L_j \sin \alpha_j \sin \beta_j \quad (14)$$

From the basic relation in fig. 6 it was straightforward to derive

$$\cos \theta_s = -\cos \theta_i \cos \psi + \sin \theta_i \sin \psi \sin \phi, \quad (15)$$

which after substitution of eqns. (11) was the same as eqn. (10) except for the fact that $\sin \phi$ appeared instead of $\cos \phi$. This difference was due to the present convention and is immaterial. One can also show that

$$\cos \phi_s = \cos \phi_i \cos(\phi_s - \phi_i) - \sin \phi_i \sin(\phi_s - \phi_i) \quad (16)$$

$$\sin \phi_s = \sin \phi_i \cos(\phi_s - \phi_i) + \cos \phi_i \sin(\phi_s - \phi_i) \quad (17)$$

where

$$\sin(\phi_s - \phi_i) = \frac{-\sin \psi \cos \phi}{\sin \theta_s} \quad (18)$$

and

$$\cos(\phi_s - \phi_i) = \frac{\sin \theta_i \cos \theta_s - \sin \psi \sin \phi}{\cos \theta_i \sin \theta_s} \quad (19)$$

Substitution of eqns. (11) and (12) then yields the required recursion relations for β_j :

$$\cos \beta_j = -\cos \beta_{j-1} \cos(\phi - \phi_i) + \sin \beta_{j-1} \sin(\phi_s - \phi_i) \quad (20)$$

$$\sin\beta_j = -\sin\beta_{j-1} \cos(\phi_s - \phi_i) - \cos\beta_{j-1} \sin(\phi_s - \phi_i) \quad (21)$$

where

$$\sin(\phi_s - \phi_i) = \frac{-\sin\psi \cos\phi}{\sin\alpha_j} \quad (22)$$

$$\cos(\phi_s - \phi_i) = \frac{\sin\psi \sin\phi - \sin\alpha_{j-1} \cos\alpha_j}{\cos\alpha_{j-1} \cos\alpha_j} \quad (23)$$

Two special cases must be tested for and treated separately: (1) $\sin\theta_s = 0$ -- in this case the projectile scatters along $\hat{z}_j$ and ϕ_s is ambiguous--TRIM: TRAJECTORY chooses $\phi_s = 0$ for this case; (2) $\sin\theta_s \neq 0$ but $\cos\theta_i = 0$ --in this case eqn. (19) yields the indeterminate ratio 0/0 and one must use

$$\cos(\phi_s - \phi_i) = -\cos\psi / \sin\alpha_j \quad (24)$$

in place of eqn. (23).

It was subsequently found possible to simplify eqn. (19) somewhat employing eqn. (15). It can be rewritten as

$$\cos(\phi_s - \phi_i) = \frac{-\sin\theta_i \cos\psi - \cos\theta_i \sin\psi \sin\phi}{\sin\theta_s} \quad (25)$$

If one does this, special case(2) is eliminated, however, this simplification was not appreciated until after the program had been coded and was not incorporated into TRIM: TRAJECTORY.

TRIM: TRAJECTORY was used to obtain figs. 1 and 2. An additional illustration is shown in fig. 7. This shows three trajectories of 300 eV ^4He on W in two views; the lower one (b) is a projection of the three-dimensional trajectory onto the $x_0 - z_0$ plane and the top one (a) onto the $x_0 - y_0$ plane.

5. TRIM: CASCADE

With a working version of TRIM: TRAJECTORY it is an exercise in logic to include a threshold for displacement and to follow out the recoil trajectories as well. For the recoil one has to use

$$\psi^* = \arctan\left(\frac{\sin\theta}{1-\cos\theta}\right) \quad (26)$$

instead of inverting eqn. 6.

At first this was accomplished by storing the values of z_j , x_j , $\cos\alpha_j$, $\sin\alpha_j$, $\cos\beta_j$ and $\sin\beta_j$ for every recoil event (or branch point) in computer memory and then returning to it after the trajectory of the projectile was plotted out. Due to the rapidly increasing degree of complexity, that is, branches on branches on branches, etc., the computer memory was soon entirely used up for all but the most trivial cases. The logic was subsequently changed to follow out each recoil event before proceeding with the incident atom--even when this atom itself was a recoil. For example, the incident atom might cause recoil event number one; the recoiling atom would then be followed until it itself caused recoil event number two. This recoiling atom would then be followed. Assume for the moment that this atom loses all its energy without causing further recoils. If so, then the coordinates of the incident atom at recoil event number two (that is, the branch index, B, equals 2) would be restored and its trajectory followed. The coordinates of this atom at the next collision which imparts a recoil energy greater than the threshold energy to its collision partner would then be used to overwrite the coordinates of the incident atom at recoil event number two. The amount of memory needed is dictated by the highest value of B attained. A flow chart of TRIM: CASCADE is included with the listing. Figure 8 illustrates its use for 1000 eV W on W with a displacement threshold energy of 45 eV, a cutoff energy of 40 eV (that is, trajectories were not followed if an atom's energy fell below 40 eV). TRIM: CASCADE simulates single self-ion irradiation. The case of fig. 8 produced 15 vacancies. The numbers are the values of B at the displacement events. The path of the projectile incident on the amorphous solid was indicated by values of B equal to one; the path of the first displaced atom was indicated by values of B equal to two along the very first trajectory branching from the trajectory of the primary, etc.

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APPENDIX A.

TRIM: LOW ENERGY

```
0010 REM TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY
0020 REM
0030 REM
0040 REM
0050 REM      PROGRAM TRIM: LOW ENERGY USING OEN AND ROBINSON ELECTRONIC
0060 REM      ENERGY LOSS AND APPLICABLE FOR EPSILON LESS THAN 10
0070 REM      AND FOR LO LESS THAN THE MEAN INTERATOMIC SPACING
0080 REM
0090 REM
0100 REM
0110 DIM M(100),N(100),E(100),F(100)
0120 DIM D(300)
0130 FOR I=1 TO 100
0140   LET M(I)=0
0150   LET N(I)=0
0160   LET E(I)=0
0170   LET F(I)=0
0180 NEXT I
0190 FOR I=1 TO 300
0200   LET D(I)=0
0210 NEXT I
0220 READ X1,P1,A1,A2,X2,P2
0230 RESTORE
0240 READ S1,S2,I1,E1
0250 LET P9=3.14159
0260 INPUT "ATOMIC NUMBER OF PROJECTILE=",Z1
0270 INPUT "MASS OF PROJECTILE=",M1
0280 INPUT "ATOMIC NUMBER OF TARGET=",Z2
0290 INPUT "MASS OF TARGET=",M2
0300 INPUT "DENSITY OF TARGET=",R1
0310 INPUT "ENERGY OF PROJECTILE=",E0
0320 INPUT "CUTOFF ENERGY=",E3
0330 INPUT "LINDHARD ELECTRONIC STOPPING CORRECTION FACTOR=",C1
0340 INPUT "BIN WIDTH=",C2
0350 INPUT "NUMBER OF ION HISTORIES=",N1
0360 LET M3=M1/M2
0370 LET A4=R1*.6022/M2
0380 LET A=.529*.8853/(Z1.5+Z2.5)(2/3)
0390 LET F1=A*M2/(Z1*Z2*14.4*(M1+M2))
0400 LET E4=E0*F1
0410 LET L1=(.02*(1+M3)2)/(4*P9*A*A*A4)
0420 LET L0=L1*(E42+.052*E41.32)/LOG(1+E4)
0430 LET L2=A4(-1/3)
0440 LET K1=1.212*Z1(7/6)*Z2/((Z1(2/3)+Z2(2/3))1.5*SQR(M1))
0450 LET K=C1*K1
0460 LET K2=.1334*Z2(2/3)/SQR(M2)
0470 LET F2=.01024/Z2(7/3)
0480 LET D(101)=K*.045/(P9*A*A)
```

```
0490 FOR I4=1 TO N1
0510   LET E6=E0
0520   LET X=0
0530   LET C3=1
0540   LET S4=0
0550   LET P3=0
0560   IF D(201)<65536 THEN GOTO 0630
0570   IF D(201)<2*65536 THEN GOTO 0610
0580   IF D(201)<3*65536 THEN GOTO 0610
0590   IF D(201)<4*65536 THEN GOTO 0630
0600   GOTO 1170
0610   LET R4=1-RND(1)
0620   GOTO 0640
0630   LET R4=RND(1)
0640   LET D(201)=D(201)+1
0650   LET E7=E6*F1
0660   LET L3=L2
0670   LET A5=L3*A4
0680   LET P=SQR(R4/A5/P9)
0690   LET B=P/A
0700   LET E9=4*M3/(1+M3)^2*E6
0710   REM CALL TO MAGIC (E7,B,C4,S8,X3)
0720   GOSUB 1780
0730   LET D3=E9*S8
0740   LET L3=L2-P*SQR(S8/C4)
0750   LET D1=D(101)*SQR(E6)*X3
0760   LET E6=E6-D3-D1
0770   LET P3=P3+L3/C2
0780   IF D(201)<65536 THEN GOTO 0850
0790   IF D(201)<2*65536 THEN GOTO 0830
0800   IF D(201)<3*65536 THEN GOTO 0850
0810   IF D(201)<4*65536 THEN GOTO 0830
0820   GOTO 1170
0830   LET R7=1-RND(1)
0840   GOTO 0860
0850   LET R7=RND(1)
0860   LET D(201)=D(201)+1
0870   LET P4=2*P9*R7
0880   LET C6=2*C4-1
0890   LET T2=SQR(1-C6*C6)
0900   LET P5=ATN(T2/(C6+M3))
0910   IF P5<0 THEN LET P5=P5+P9
0920   LET C3=C3*COS(P5)+S4*SIN(P5)*COS(P4)
0930   LET S4=SQR(1-C3*C3)
0940   LET X=X+L3*C3
0950   IF X<0 THEN GOTO 1130
0960   LET I=INT(X/C2+1)
0970   IF I>100 THEN LET I=100
0980   LET E(I)=E(I)+D1
0990   LET F(I)=F(I)+D3
1000   LET P6=F2*D3
1010   LET G=P6+.40244*P6^(.75)+3.4008*P6^(.1667)
1020   LET D(I)=D(I)+D3/(1+K2*G)
1030   IF E6>E3 THEN GOTO 0560
```

```
1040 LET M(I)=M(I)+1
1050 LET I5=INT(P3+1)
1060 IF I5>100 THEN LET I5=100
1070 LET N(I5)=N(I5)+1
1080 LET X1=X1+X
1090 LET P1=P1+P3*C2
1100 LET X2=X2+X^2
1110 LET P2=P2+(P3*C2)^2
1120 GOTO 1150
1130 LET I1=I1+1
1140 LET E1=E1+E6
1150 NEXT I4
1160 GOTO 1210
1170 PRINT
1180 PRINT
1190 PRINT "MACRANDER RANDOM NUMBER CAPACITY HAS BEEN REACHED"
1200 LET N1=I4-1
1210 PRINT
1220 PRINT
1222 PRINT
1223 PRINT "TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY"
1224 PRINT
1225 PRINT
1226 PRINT "      MONTE CARLO PROGRAM TO CALCULATE IMPLANTED RANGE"
1227 PRINT "      PROFILES USING THE OEN AND ROBINSON EXPRESSION"
1228 PRINT "      FOR THE ELECTRONIC ENERGY LOSS. THIS VERSION IS"
1229 PRINT "      APPLICABLE FOR EPSILON LESS THAN 10 AND LO LESS THAN"
1230 PRINT "      THE MEAN INTERATOMIC SPACING"
1231 PRINT "      VERSION: 11/10/78"
1232 PRINT
1233 PRINT
1250 PRINT "TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY TRIM: LOW ENERGY"
1252 PRINT
1253 PRINT
1260 PRINT "NUMBER OF RANDOM NUMBERS USED=";D(201)
1270 PRINT "PROJECTILE Z=";Z1,"PROJECTILE MASS=";M1
1280 PRINT "TARGET Z=";Z2,"TARGET MASS=";M2
1290 PRINT "TARGET DENSITY=";R1
1300 PRINT "ENERGY OF PROJECTILE=";E0,"CUTOFF ENERGY=";E3
1310 PRINT "EPSILON=";E4
1320 PRINT "MEAN INTERATOMIC SPACING=";L2,"LO=";LO
1330 PRINT "LINDHARD ELECTRONIC STOPPING CORRECTION FACTOR=";C1
1340 PRINT
1350 PRINT
1360 PRINT "NUMBER OF PARTICLES BACKSCATTERED=";I1
1370 PRINT "ENERGY=";E1
1380 IF X1=0 THEN GOTO 1460
1390 LET H1=N1-I1
1400 LET A1=X1/H1
1410 LET A2=P1/H1
1420 LET S1=SQR((X2-H1*A1^2)/H1)
1430 LET S2=SQR((P2-H1*A2^2)/H1)
1440 PRINT
1450 PRINT
```

```

1460 PRINT "AVERAGE PROJECTED RANGE=",A1
1470 PRINT "STANDARD DEVIATION=",S1
1480 PRINT
1490 PRINT
1500 PRINT "AVERAGE TOTAL PATHLENGTH=",A2
1510 PRINT "STANDARD DEVIATION=",S2
1520 PRINT
1530 PRINT
1540 PRINT "FIRST TWO COLUMNS DENOTE DEPTH IN ANGSTROMS"
1550 PRINT "THIRD COLUMN DENOTES THE NUMBER OF PARTICLES IN EACH BIN"
1560 PRINT "FOURTH COLUMN DENOTES THE NUMBER OF PARTICLES WITH"
1570 PRINT "A GIVEN TOTAL PATHLENGTH"
1580 PRINT "THE FIFTH COLUMN GIVES THE ELECTRONIC ENERGY LOSS"
1590 PRINT "THE SIXTH COLUMN GIVES THE NUCLEAR ENERGY LOSS"
1600 PRINT "THE LAST COLUMN GIVES THE DAMAGE ENERGY CALCULATED FROM"
1610 PRINT "THE ENERGY LOST TO RECOILS"
1620 PRINT
1630 LET D4=0
1640 LET D5=C2
1650 FOR J=1 TO 100
1660   IF N(101-J)<>0 THEN GOTO 1680
1670 NEXT J
1680 LET D(199)=102-J
1690 IF D(199)>100 THEN LET D(199)=100
1700 FOR J=1 TO D(199)
1710   PRINT D4;D5;M(J);N(J);E(J);F(J);D(J)
1720   LET D4=D5
1730   LET D5=D5+C2
1740 NEXT J
1750 STOP
1760 END
1770 DATA 0,0,0,0,0,0
1780 REM SUBROUTINE MAGIC (E7,B,C4,S8,X3)
1790 LET R=B
1800 LET R5=LOG(.35/(E7*B))/ .3
1810 IF R5<B THEN GOTO 1850
1820 LET R5=LOG(.35/(E7*R5))/ .3
1830 IF R5<B THEN GOTO 1850
1840 LET R=R5
1850 LET X3=EXP(-.3*R)
1860 LET X4=X3^4
1870 LET X5=X4^5
1880 LET V=(.35*X3+.55*X4+.1*X5)/R
1890 LET F3=B*B/R+V*R/E7 R
1900 LET R0=-(V+.105*X3+.66*X4+.6*X5)/R
1910 LET R2=-B*B/(R*R)+(V+R0*R)/E7-1
1920 LET J=F3/R2
1930 LET R=R-J
1940 IF ABS(J/R)>.001 THEN GOTO 1850
1950 LET A1=-2*(E7-V)/R0
1960 LET A2=SQR(E7)
1970 LET R5=(.009611+A2)/(.005175+A2)
1980 LET S1=2*E7*(1+(.6743/A2))*B^R5
1990 LET S2=(SQR(S1^2+1)-S1)*((6.314+E7)/(10+E7))

```

```
2000 LET C4=(R-B)*S1*S2/(S2+1)
2010 LET S8=(B+C4+A1)/(R+A1)
2020 LET C4=S8*S8
2030 LET S8=1-C4
2040 RETURN
```

APPENDIX B.

TRIM: ALLOY

```
0010 REM TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY
0020 REM
0030 REM          ALLOY VERSION: 11/11/78
0040 REM
0050 REM          PROGRAM TRIM: ALLOY USING OEN AND ROBINSON ELECTRONIC
0060 REM          ENERGY LOSS AND APPLICABLE FOR EPSILON LESS THAN 10
0070 REM          AND FOR LO LESS THAN THE MEAN INTERATOMIC SPACING
0080 REM
0090 REM
0100 REM
0110 DIM N(100),E(100),F(100)
0120 DIM D(300),M(300)
0130 FOR I=1 TO 100
0140   LET M(I)=0
0150   LET N(I)=0
0160   LET E(I)=0
0170   LET F(I)=0
0180 NEXT I
0190 FOR I=1 TO 300
0200   LET D(I)=0
0210   LET M(I)=0
0220 NEXT I
0230 READ X1,P1,A1,A2,X2,P2
0240 RESTORE
0250 READ S1,S2,I1,E1
0260 LET P9=3.14159
0270 PRINT
0280 PRINT
0290 PRINT "TRIM: ALLOY"
0300 PRINT "  ALLOY VERSION: 11/11/78"
0310 PRINT
0320 INPUT "ATOMIC NUMBER OF PROJECTILE=",Z1
0330 INPUT "MASS OF PROJECTILE=",M1
0340 INPUT "  RATIO (FOR PT3CO IT IS 4)=",D(250)
0350 INPUT "Z OF THE MAIN COMPONENT OF THE TARGET=",D(191)
0360 INPUT "Z OF THE MINOR COMPONENT=",D(192)
0370 INPUT "MASS OF THE MAIN COMPONENT=",M(101)
0380 INPUT "MASS OF THE MINOR COMPONENT=",M(102)
0390 INPUT "DENSITY OF TARGET=",R1
0400 INPUT "ENERGY OF PROJECTILE=",E0
0410 INPUT "CUTOFF ENERGY=",E3
0420 INPUT "LINDHARD ELECTRONIC STOPPING CORRECTION FACTOR=",C1
0430 INPUT "BIN WIDTH=",C2
0440 INPUT "NUMBER OF ION HISTORIES=",N1
0450 LET A4=R1*.6022/((D(250)-1)*M(101)/D(250)+M(102)/D(250))
0460 LET L2=A4^(-1/3)
0470 FOR I=1 TO 2
0480   LET M(200+I)=M1/M(100+I)
```



```

0490 LET M(110+I)=.529*.8853/(SQR(Z1)+SQR(D(190+I)))^(2/3)
0500 LET M(120+I)=M(110+I)*M(100+I)/(Z1*D(190+I)*14.4*(M1+M(100+I)))
0510 LET M(130+I)=E0*M(120+I)
0520 LET M(140+I)=(.02*(1+M(200+I))^2)/(4*P9*M(110+I)^2*A4)
0530 LET M(150+I)=M(140+I)*(M(130+I)^2+.052*M(130+I)^1.32)/LOG(1+M(130+I))
0540 LET M(160+I)=1.212*Z1^(7/6)*D(190+I)/((Z1^(2/3)+D(190+I)^(2/3))^1.5*SQR(M
1))
0550 LET M(170+I)=C1*M(160+I)
0560 LET M(180+I)=.1334*D(190+I)^(2/3)/SQR(M(100+I))
0570 LET M(190+I)=.01024/D(190+I)^(7/3)
0580 LET D(100+I)=M(170+I)*.045/(P9*M(110+I)^2)
0590 NEXT I
0600 FOR I4=1 TO N1
0610 LET E6=E0
0620 LET X=0
0630 LET C3=1
0640 LET S4=0
0650 LET P3=0
0660 IF D(201)<65536 THEN GOTO 0730
0670 IF D(201)<2*65536 THEN GOTO 0710
0680 IF D(201)<3*65536 THEN GOTO 0710
0690 IF D(201)<4*65536 THEN GOTO 0730
0700 GOTO 1330
0710 LET R4=1-RND(1)
0720 GOTO 0740
0730 LET R4=RND(1)
0740 LET D(201)=D(201)+1
0750 LET R5=RND(1)
0760 LET D(201)=D(201)+1
0770 IF R5<((1/D(250))) THEN GOTO 0800
0780 LET X0=1
0790 GOTO 0810
0800 LET X0=2
0810 LET E7=E6*M(120+X0)
0820 LET L3=L2
0830 LET A5=L3*A4
0840 LET P=SQR(R4/A5/P9)
0850 LET B=P/M(110+X0)
0860 LET E9=4*M(200+X0)/(1+M(200+X0))^2*E6
0870 REM CALL TO MAGIC (E7,B,C4,S8,X3)
0880 GOSUB 2270
0890 LET D3=E9*S8
0900 LET L3=L2-P*SQR(S8/C4)
0910 LET D1=D(100+X0)*SQR(E6)*X3
0920 LET E6=E6-D3-D1
0930 LET P3=P3+L3/C2
0940 IF D(201)<65536 THEN GOTO 1010
0950 IF D(201)<2*65536 THEN GOTO 0990
0960 IF D(201)<3*65536 THEN GOTO 1010
0970 IF D(201)<4*65536 THEN GOTO 0990
0980 GOTO 1330
0990 LET R7=1-RND(1)
1000 GOTO 1020
1010 LET R7=RND(1)

```

```

1020 LET D(201)=D(201)+1
1030 LET P4=2*P9*R7
1040 LET C6=2*C4-1
1050 LET T2=SQR(1-C6*C6)
1060 LET P5=ATN(T2/(C6+M(200+X0)))
1070 IF P5<0 THEN LET P5=P5+P9
1080 LET C3=C3*COS(P5)+S4*SIN(P5)*COS(P4)
1090 LET S4=SQR(1-C3*C3)
1100 LET X=X+L3*C3
1110 IF X<0 THEN GOTO 1290
1120 LET I=INT(X/C2+1)
1130 IF I>100 THEN LET I=100
1140 LET E(I)=E(I)+D1
1150 LET F(I)=F(I)+D3
1160 LET P6=D3*M(190+X0)
1170 LET G=P6+.40244*P6^(.75)+3.4008*P6^(.1667)
1180 LET D(I)=D(I)+D3/(1+G*M(180+X0))
1190 IF E6>E3 THEN GOTO 0660
1200 LET M(I)=M(I)+1
1210 LET I5=INT(P3+1)
1220 IF I5>100 THEN LET I5=100
1230 LET N(I5)=N(I5)+1
1240 LET X1=X1+X
1250 LET P1=P1+P3*C2
1260 LET X2=X2+X^2
1270 LET P2=P2+(P3*C2)^2
1280 GOTO 1310
1290 LET I1=I1+1
1300 LET E1=E1+E6
1310 NEXT I4
1320 GOTO 1370
1330 PRINT
1340 PRINT
1350 PRINT "MACRANDER RANDOM NUMBER CAPACITY HAS BEEN REACHED"
1360 LET N1=I4-1
1370 PRINT
1380 PRINT
1390 PRINT
1400 PRINT "TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: AL
LOY"
1410 PRINT
1420 PRINT
1430 PRINT " MONTE CARLO PROGRAM TO CALCULATE IMPLANTED RANGE"
1440 PRINT " PROFILES USING THE OEN AND ROBINSON EXPRESSION"
1450 PRINT " FOR THE ELECTRONIC ENERGY LOSS. THIS VERSION IS"
1460 PRINT " APPLICABLE FOR EPSILON LESS THAN 10 AND LO LESS THAN"
1470 PRINT " THE MEAN INTERATOMIC SPACING"
1480 PRINT " ALLOY VERSION: 11/11/78"
1490 PRINT
1500 PRINT
1510 PRINT "TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: ALLOY TRIM: AL
LOY"
1520 PRINT
1530 PRINT

```

```
1540 PRINT "NUMBER OF RANDOM NUMBERS USED=";D(201)
1550 PRINT "PROJECTILE Z=";Z1,"PROJECTILE MASS=";M1
1560 PRINT "RATIO=";D(250)
1570 PRINT "MAIN COMPONENT OF THE TARGET: Z=";D(191),"MASS=";M(101)
1580 PRINT "MINOR COMPONENT: Z=";D(192),"MASS=";M(102)
1590 PRINT "TARGET DENSITY=";R1
1600 PRINT "ENERGY OF PROJECTILE=";E0,"CUTOFF ENERGY=";E3
1610 PRINT "EPSILON (MAIN COMPONENT)=";M(131)
1620 PRINT "EPSILON (MINOR COMPONENT)=";M(132)
1630 PRINT "MEAN INTERATOMIC SPACING=";L2
1640 PRINT "LO (MAIN COMPONENT)=";M(151)
1650 PRINT "LO (MINOR COMPONENT)=";M(152)
1660 PRINT "LINDHARD ELECTRONIC STOPPING CORRECTION FACTOR=";C1
1670 PRINT
1680 PRINT
1690 PRINT "NUMBER OF PARTICLES BACKSCATTERED=";I1
1700 PRINT "ENERGY=";E1
1710 IF X1=0 THEN GOTO 1860
1720 LET H1=N1-I1
1730 LET A1=X1/H1
1740 LET A2=P1/H1
1750 LET S1=SQR((X2-H1*A1^2)/H1)
1760 LET S2=SQR((P2-H1*A2^2)/H1)
1770 FOR I=1 TO 100
1780 LET D(150)=D(150)+D(I)*(I-.5)*C2
1790 LET D(152)=D(152)+D(I)*((I-.5)*C2)^2
1800 LET D(154)=D(154)+D(I)
1810 NEXT I
1820 LET D(155)=D(150)/D(154)
1830 LET D(163)=SQR((D(152)-D(154)*D(155)^2)/D(154))
1840 PRINT
1850 PRINT
1860 PRINT "AVERAGE PROJECTED RANGE=";A1
1870 PRINT "STANDARD DEVIATION=";S1
1880 PRINT
1890 PRINT
1900 PRINT "AVERAGE TOTAL PATHLENGTH=";A2
1910 PRINT "STANDARD DEVIATION=";S2
1920 PRINT
1930 PRINT
1940 PRINT "AVERAGE DAMAGE DEPTH=";D(155)
1950 PRINT "STANDARD DEVIATION=";D(163)
1960 PRINT
1970 PRINT
1980 PRINT "FIRST TWO COLUMNS DENOTE DEPTH IN ANGSTROMS"
1990 PRINT "THIRD COLUMN DENOTES THE NUMBER OF PARTICLES IN EACH BIN"
2000 PRINT "FOURTH COLUMN DENOTES THE NUMBER OF PARTICLES WITH"
2010 PRINT "A GIVEN TOTAL PATHLENGTH"
2020 PRINT "THE FIFTH COLUMN GIVES THE ELECTRONIC ENERGY LOSS"
2030 PRINT "THE SIXTH COLUMN GIVES THE NUCLEAR ENERGY LOSS"
2040 PRINT "THE SEVENTH COLUMN GIVES THE DAMAGE ENERGY CALCULATED"
2050 PRINT "FROM THE ENERGY LOST TO RECOILS."
2060 PRINT "THE LAST COLUMN GIVES THE REDUCED DAMAGE ENERGY"
2070 PRINT
```

```
2080 LET D4=0
2090 LET D5=C2
2100 FOR J=1 TO 100
2110 IF N(101-J)<>0 THEN GOTO 2130
2120 NEXT J
2130 LET A=0
2140 FOR I=1 TO 100
2150 IF D(I)>A THEN LET A=D(I)
2160 NEXT I
2170 LET D(199)=102-J
2180 IF D(199)>100 THEN LET D(199)=100
2190 FOR J=1 TO D(199)
2200 PRINT D4;D5;M(J);N(J);E(J);F(J);D(J);D(J)/A
2210 LET D4=D5
2220 LET D5=D5+C2
2230 NEXT J
2240 STOP
2250 END
2260 DATA 0,0,0,0,0,0
2270 REM SUBROUTINE MAGIC (E7,B,C4,S8,X3)
2280 LET R=B
2290 LET R5=LOG(.35/(E7*B))/.3
2300 IF R5<B THEN GOTO 2340
2310 LET R5=LOG(.35/(E7*R5))/.3
2320 IF R5<B THEN GOTO 2340
2330 LET R=R5
2340 LET X3=EXP(-.3*R)
2350 LET X4=X3^4
2360 LET X5=X4^5
2370 LET V=(.35*X3+.55*X4+.1*X5)/R
2380 LET F3=B*B/R+V*R/E7-R
2390 LET R0=-(V+.105*X3+.66*X4+.6*X5)/R
2400 LET R2=-B*B/(R*R)+(V+R0*R)/E7-1
2410 LET J=F3/R2
2420 LET R=R-J
2430 IF ABS(J/R)>.001 THEN GOTO 2340
2440 LET A1=-2*(E7-V)/R0
2450 LET A2=SQR(E7)
2460 LET R5=(.009611+A2)/(.005175+A2)
2470 LET S1=2*E7*(1+(.6743/A2))*B^R5
2480 LET S2=(SQR(S1^2+1)-S1)*((6.314+E7)/(10+E7))
2490 LET C4=(R-B)*S1*S2/(S2+1)
2500 LET S8=(B+C4+A1)/(R+A1)
2510 LET C4=S8*S8
2520 LET S8=1-C4
2530 RETURN
```

APPENDIX C.

TRIM: TRAJECTORY

```
0010 REM PROGRAM TRIM: TRAJECTORY
0015 REM TRAJECTORIES, SHORTENED VERSION
0016 REM 04/06/79
0020 DIM M(100),N(100),E(100),F(100)
0025 DIM D(300)
0030 FOR I=1 TO 100
0040   LET M(I)=0
0050   LET N(I)=0
0060   LET E(I)=0
0070   LET F(I)=0
0090 NEXT I
0091 FOR I=1 TO 300
0092   LET D(I)=0
0093 NEXT I
0100 READ X1,F1,A1,A2,X2,P2
0110 RESTORE
0120 READ S1,S2,I1,I2,E1,E2
0130 LET P9=3.14159
0135 PRINT "Z1,M1,Z2,M2,R1"
0140 INPUT Z1,M1,Z2,M2,R1
0145 PRINT "E0,E3,C1"
0150 INPUT E0,E3,C1
0160 INPUT "N1 ",N1
0161 INPUT "SCALE FACTOR=",D(200)
0180 LET M3=M1/M2
0190 LET A4=R1*.6022/M2
0200 LET A=.529*.8853/(Z1^.5+Z2^.5)^(2/3)
0210 LET F1=A*M2/(Z1*Z2*14.4*(M1+M2))
0220 LET E4=E0*F1
0230 LET L1=(.02*(1+M3)^2)/(4*P9*A*A*A4)
0240 LET L0=L1*(E4^2+.052*E4^1.32)/LOG(1+E4)
0250 LET L2=A4^(-1/3)
0260 LET K1=1.212*Z1^(7/6)*Z2/((Z1^(2/3)+Z2^(2/3))^1.5*SQR(M1))
0270 LET K=C1*K1
0280 LET K2=.1334*Z2^(2/3)/SQR(M2)
0290 LET F2=.01024/Z2^(7/3)
0331 LET D(101)=K*.045/(P9*A*A)
0340 FOR I4=1 TO N1
0350   LET E6=E0
0360   LET X=0
0365   LET X0=0
0370   LET C3=1
0375   LET A3=-1
0380   LET S4=0
0385   LET T1=0
0410   LET R3=RND(1)
0420   LET R4=RND(1)
0430   LET E7=E6*F1
```

```
0610 LET L3=L2
0620 LET A5=L3*A4
0670 LET P=SQR(R4/A5/P9)
0680 LET B=P/A
0690 LET E9=4*M3/(1+M3)^2*E6
0740 GOSUB 6000
0750 LET D3=E9*S8
0751 LET L3=L2-P*SQR(S8/C4)
0752 LET D1=D(101)*SQR(E6)*X3
0760 LET E6=E6-D3-D1
0780 LET R7=RND(1)
0790 LET P4=2*P9*R7
0800 LET C6=2*C4-1
0810 LET T2=SQR(1-C6*C6)
0820 LET P5=ATN(T2/(C6+M3))
0821 IF P5<0 THEN LET P5=P5+P9
0824 LET S1=C3
0825 LET A1=S4
0826 LET C3=C3*COS(P5)+S4*SIN(P5)*SIN(P4)
0827 LET S4=SQR(1-C3*C3)
0828 IF S4<>0 THEN GOTO 0832
0829 LET A3=1
0830 LET T1=0
0831 GOTO 0840
0832 IF S1<>0 THEN GOTO 0835
0833 LET C6=-COS(P5)/S4
0834 GOTO 0836
0835 LET C6=(SIN(P5)*SIN(P4)-A1*C3)/(S1*S4)
0836 LET T2=-SIN(P5)*COS(P4)/S4
0837 LET S1=-A3*C6+T1*T2
0838 LET T1=-T1*C6-A3*T2
0839 LET A3=S1
0840 LET A1=X
0850 LET X=X+L3*C3
0851 LET S1=X0
0855 LET X0=X0+L3*A3*S4
0856 CALL 20,D(200)*A1,400+D(200)*S1,D(200)*X,400+D(200)*X0
0860 IF X<0 THEN GOTO 1100
0870 IF X>1000/D(200) THEN GOTO 1100
0871 IF X0>500/D(200) THEN GOTO 1100
0872 IF X0<-500/D(200) THEN GOTO 1100
0950 IF E6>E3 THEN GOTO 0420
1100 NEXT I4
1104 CALL 20,1000,0,1000,100
1105 STOP
1420 END
5000 DATA 0,0,0,0,0,0
6000 REM SUBROUTINE MAGIC (E7,B,C4,S8)
6010 LET R=B
6020 LET R5=LOG(.35/(E7*B))/.3
6024 IF R5<B THEN GOTO 6050
6028 LET R5=LOG(.35/(E7*R5))/.3
6030 IF R5<B THEN GOTO 6050
6040 LET R=R5
```



```
6050 LET X3=EXP(-.3*R)
6060 LET X4=X3^4
6070 LET X5=X4^5
6080 LET V=(.35*X3+.55*X4+.1*X5)/R
6090 LET F3=B*B/R+V*R/E7-R
6100 LET R0=-(V+.105*X3+.66*X4+.6*X5)/R
6110 LET R2=-B*B/(R*R)+(V+R0*R)/E7-1
6120 LET J=F3/R2
6130 LET R=R-J
6140 IF ABS(J/R)>.001 THEN GOTO 6050
6150 LET A1=-2*(E7-V)/R0
6160 LET A2=SQR(E7)
6170 LET R5=(.009611+A2)/(.005175+A2)
6180 LET S1=2*E7*(1+(.6743/A2))*B^R5
6190 LET S2=(SQR(S1^2+1)-S1)*((6.314+E7)/(10+E7))
6200 LET C4=(R-B)*S1*S2/(S2+1)
6210 LET S8=(B+C4+A1)/(R+A1)
6220 LET C4=S8*S8
6230 LET S8=1-C4
6240 RETURN
```

APPENDIX D.

TRIM: CASCADE

```
0005 RANDOMIZE
0010 REM TRIM: CASCADE MARCH 2,1979
0020 DIM E(110)
0030 DIM F(300),D(300),M(300)
0040 DIM N(400)
0060 FOR I=1 TO 110
0070   LET E(I)=0
0100 NEXT I
0110 FOR I=1 TO 300
0120   LET D(I)=0
0130   LET F(I)=0
0131   LET M(I)=0
0140 NEXT I
0150 FOR I=1 TO 400
0160   LET N(I)=0
0170 NEXT I
0180 LET P9=3.14159
0190 INPUT "ATOMIC NUMBER=",Z1
0200 INPUT "MASS=",M1
0210 INPUT "DENSITY=",R1
0220 INPUT "ENERGY=",E0
0230 INPUT "CUTOFF ENERGY=",E3
0240 INPUT "LINDHARD ELECTRONIC STOPPING CORRECTION FACTOR=",C1
0250 INPUT "THRESHOLD ENERGY=",M(102)
0260 INPUT "SCALE FACTOR=",D(300)
0270 LET M2=M1
0280 LET Z2=Z1
0290 LET M3=M1/M2
0300 LET A4=R1*.6022/M2
0310 LET A=.529*.8853/(Z1.5+Z2.5)(2/3)
0320 LET F1=A*M2/(Z1*Z2*14.4*(M1+M2))
0330 LET E4=E0*F1
0340 LET L1=(.02*(1+M3)2)/(4*P9*A*A*A4)
0350 LET L0=L1*(E42+.052*E41.32)/LOG(1+E4)
0360 LET L2=A4(-1/3)
0370 LET K1=1.212*Z1(7/6)*Z2/((Z1(2/3)+Z2(2/3))1.5*SQR(M1))
0380 LET K=C1*K1
0390 LET K2=.1334*Z2(2/3)/SQR(M2)
0400 LET F2=.01024/Z2(7/3)
0410 LET D(101)=K*.045/(P9*A*A)
0420 LET E6=E0
0430 LET X=0
0440 LET X0=0
0450 LET C3=1
0460 LET A3=-1
0470 LET S4=0
0480 LET T1=0
0490 LET R4=RND(1)
```

```
0500 LET D(201)=D(201)+1
0510 LET E7=E6*F1
0520 LET L3=L2
0530 LET A5=L3*A4
0540 LET P=SQR(R4/A5/P9)
0550 LET B=P/A
0560 LET E9=4*M3/(1+M3)^2*E6
0570 REM CALL TO MAGIC (E7,B,C4,S8,X3)
0580 GOSUB 1640
0590 LET D3=E9*S8
0600 LET L3=L2-P*SQR(S8/C4)
0610 LET D1=D(101)*SQR(E6)*X3
0620 LET E6=E6-D3-D1
0621 IF E6<0 THEN GOTO 1490
0630 IF D3>M(102) THEN GOTO 0650
0640 IF E6<E3 THEN GOTO 1490
0650 LET R7=RND(1)
0660 LET D(201)=D(201)+1
0670 LET C6=2*C4-1
0680 LET T2=SQR(1-C6*C6)
0690 LET P5=ATN(T2/(C6+M3))
0700 IF P5<0 THEN LET P5=P5+P9
0710 LET P4=2*P9*R7
0720 LET E(101)=C3
0730 LET E(102)=S4
0740 LET S1=C3
0750 LET A1=S4
0760 LET C3=C3*COS(P5)+S4*SIN(P5)*SIN(P4)
0770 LET S4=SQR(1-C3*C3)
0780 LET M(103)=C3
0790 LET M(104)=S4
0800 IF S4<>0 THEN GOTO 0840
0810 LET A3=1
0820 LET T1=0
0830 GOTO 0940
0840 IF S1<>0 THEN GOTO 0870
0850 LET C6=-COS(P5)/S4
0860 GOTO 0880
0870 LET C6=(SIN(P5)*SIN(P4)-A1*C3)/(S1*S4)
0880 LET T2=-SIN(P5)*COS(P4)/S4
0890 LET E(103)=A3
0900 LET E(104)=T1
0910 LET S1=-A3*C6+T1*T2
0920 LET T1=-T1*C6-A3*T2
0930 LET A3=S1
0940 LET M(105)=A3
0950 LET M(106)=T1
0960 LET M(107)=X
0970 LET X=X+L3*C3
0980 LET M(108)=X0
0990 LET X0=X0+L3*A3*S4
1000 CALL 20,D(300)*M(107),400+D(300)*M(108),D(300)*X,400+D(300)*X0
1010 IF X<0 THEN GOTO 1490
1020 IF X>1000/D(300) THEN GOTO 1490
```

```
1030 IF X0>500/D(300) THEN GOTO 1490
1040 IF X0<-500/D(300) THEN GOTO 1490
1050 IF D3<M(102) THEN GOTO 0490
1060 LET M(101)=M(101)+1
1065 LET D(202)=D(202)+1
1066 CALL 20,D(300)*M(107),400+D(300)*M(108),D(300)*M(107),400+D(300)*M(108)
1067 PRINT M(101)
1070 LET J=100+10*(M(101)-1)
1080 LET N(J+1)=M(103)
1090 LET N(J+2)=M(104)
1100 LET N(J+3)=M(105)
1110 LET N(J+4)=M(106)
1120 LET N(J+5)=X
1130 LET N(J+6)=X0
1140 LET N(J+7)=E6
1150 LET C3=E(101)
1160 LET S4=E(102)
1170 LET A3=E(103)
1180 LET T1=E(104)
1190 LET C6=2*C4-1
1200 LET T2=SQR(1-C6*C6)
1210 LET P5=ATN(T2/(1-C6))
1220 IF P5<0 THEN LET P5=P5+P9
1230 LET P4=2*P9*R7+P9
1240 LET S1=C3
1250 LET A1=S4
1260 LET C3=C3*COS(P5)+S4*SIN(P5)*SIN(P4)
1270 LET S4=SQR(1-C3*C3)
1280 IF S4<>0 THEN GOTO 1320
1290 LET A3=1
1300 LET T1=0
1310 GOTO 1400
1320 IF S1<>0 THEN GOTO 1350
1330 LET C6=-COS(P5)/S4
1340 GOTO 1360
1350 LET C6=(SIN(P5)*SIN(P4)-A1*C3)/(S1*S4)
1360 LET T2=-SIN(P5)*COS(P4)/S4
1370 LET S1=-A3*C6+T1*T2
1380 LET T1=-T1*C6-A3*T2
1390 LET A3=S1
1400 LET X=M(107)+L3*C3
1410 LET X0=M(108)+L3*A3*S4
1420 CALL 20,D(300)*M(107),400+D(300)*M(108),D(300)*X,400+D(300)*X0
1430 IF X<0 THEN GOTO 1490
1440 IF X>1000/D(300) THEN GOTO 1490
1450 IF X>500/D(300) THEN GOTO 1490
1460 IF X0<-500/D(300) THEN GOTO 1490
1470 LET E6=D3
1480 GOTO 0490
1490 IF M(101)=0 THEN GOTO 1600
1500 LET J=100+10*(M(101)-1)
1510 LET C3=N(J+1)
1520 LET S4=N(J+2)
1530 LET A3=N(J+3)
```

```
1540 LET T1=N(J+4)
1550 LET X=N(J+5)
1560 LET X0=N(J+6)
1570 LET E6=N(J+7)
1580 LET M(101)=M(101)-1
1590 GOTO 0490
1600 CALL 20,1000,0,1000,100
1601 CALL 20,700,0,700,0
1610 PRINT 1000/D(300);"ANGSTROMS"
1620 STOP
1630 REM SUBROUTINE MAGIC
1640 LET R=B
1650 LET R5=LOG(.35/(E7*B))/.3
1660 IF R5<B THEN GOTO 1700
1670 LET R5=LOG(.35/(E7*R5))/.3
1680 IF R5<B THEN GOTO 1700
1690 LET R=R5
1700 LET X3=EXP(-.3*R)
1710 LET X4=X3^4
1720 LET X5=X4^5
1730 LET V=(.35*X3+.55*X4+.1*X5)/R
1740 LET F3=B*B/R+V*R/E7-R
1750 LET R0=-(V+.105*X3+.66*X4+.6*X5)/R
1760 LET R2=-B*B/(R*R)+(V+R0*R)/E7-1
1770 LET J=F3/R2
1780 LET R=R-J
1790 IF ABS(J/R)>.001 THEN GOTO 1700
1800 LET A1=-2*(E7-V)/R0
1810 LET A2=SQR(E7)
1820 LET R5=(.009611+A2)/(.005175+A2)
1830 LET S1=2*E7*(1+(.6743/A2))*B^R5
1840 LET S2=(SQR(S1^2+1)-S1)*((6.314+E7)/(10+E7))
1850 LET C4=(R-B)*S1*S2/(S2+1)
1860 LET S8=(B+C4+A1)/(R+A1)
1870 LET C4=S8*S8
1880 LET S8=1-C4
1890 RETURN
```

Flow Chart for TRIM: CASCADE

Table: Scheme used to extend random number generator supplied with NOVA
1220 minicomputer

Number of random numbers used	P	ϕ
1 - 65535	RND	RND
65536 - 2*65535	1-RND	1-RND
2*65535+1 - 3*65535	1-RND	RND
3*65535+1 - 4*65535	RND	1-RND

FIGURE CAPTIONS

- Figure 1. Ten trajectories of 30 keV W on W. Trajectories were followed until the energy fell below 1 eV. This figure was made using TRIM: TRAJECTORY and is included here to show the general lack of backscattered events (events for which $\psi > \pi/2$) for this case. All ten projectiles were implanted.
- Figure 2. Ten trajectories of 500 eV ^4He on W. Trajectories were followed until the energy fell below 1 eV. This figure was produced using TRIM: TRAJECTORY and is included here to show the importance of backscattered events (events for which $\psi > \pi/2$) for this case. Seven projectiles were backreflected (indicated by the letter b) and three were implanted.
- Figure 3. Projected range and total pathlength distributions for 300 eV ^4He on W. Mean values are indicated. The straggling of the projected range distribution was $22.3 \text{ \AA}$, and the straggling of the total pathlength distribution was $25.9 \text{ \AA}$. These distributions are for 340 implanted events out of 1000 histories followed. The ^4He particles were followed until their energy fell below 1 eV.
- Figure 4. Total nuclear and electronic energy loss distributions for the same case as figure 3 (^4He on W). These distributions are the accumulated energy lost by all 1000 ^4He particles in $5 \text{ \AA}$ wide bins located at given depths below the surface. The energy loss distributions include the energy lost by the 660 backreflected particles while they were inside the target.
- Figure 5. The fraction of particles backreflected (R_N) and the fraction of energy backreflected (R_E) for ^1H on W and for ^4He on W versus reduced energy, ϵ .
- Figure 6. Reference frames, coordinates of unit vectors, and basic relations used in deriving the recursion relations which are used in TRIM: TRAJECTORY. The $(\hat{x}_0, \hat{y}_0, \hat{z}_0)$ frame is fixed in the target. The surface of the target

is parallel to the x_0-y_0 plane and $\hat{z}_0$ points into the target. The $(\hat{x}, \hat{y}, \hat{z})$ frame is chosen so that $\hat{x}$ lies in the x_0-y_0 plane and the incident direction, $\hat{i}$, is equal to $-\hat{z}$. θ_i and θ_s are the polar angles of $-\hat{i}$ and the scattering direction, $\hat{s}$, respectively, and ϕ_i and ϕ_s are the azimuthal angles.

Figure 7. Two views of the same three trajectories of 300 eV ^4He projectiles on W. View (a) is from a vantage point which sites along the incident direction, and view (b) is in cross section. Figures 1, 2 and 9 all correspond to view (b).

Figure 8. A trajectory plot of a single 1 keV W on W trajectory with the accompanying displaced atom trajectories. The trajectories of all atoms receiving at least 45 eV in recoil energy were followed until their energy fell below 40 eV. The path of the incident projectile is indicated by values of the branch index equal to one. This plot was generated using TRIM: CASCADE.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Basic relations:

- i)
$$\cos \psi = \hat{s} \cdot \hat{z} = -\sin \theta_i \cos \phi_i \sin \theta_s \cos \phi_s - \sin \theta_i \sin \phi_i \sin \theta_s \sin \phi_s - \cos \theta_i \cos \theta_s$$
- ii)
$$\sin \psi \cos \phi = \hat{s} \cdot \hat{x} = \sin \phi_i \sin \theta_s \cos \phi_s - \cos \phi_i \sin \theta_s \sin \phi_s$$
- iii)
$$\sin \psi \sin \phi = \hat{s} \cdot \hat{y} = -\cos \theta_i \cos \phi_i \sin \theta_s \cos \phi_s - \cos \theta_i \sin \phi_i \sin \theta_s \sin \phi_s + \sin \theta_i \cos \theta_s$$

Figure 6

300 eV ^4He on W

For view (a), the surface is parallel to the plane of the paper.

(a)

100 Å

Point of Entry

Surface

b b

$\hat{x}_0$

$\hat{z}_0$

(b)

100 Å
DEPTH

Figure 7

Figure 8