User's Manual for "HERAD" - "Heterogeneous Radiation Damage" Monte Carlo Computer Code

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"Heterogeneous Radiation Damage" Monte Carlo Computer Code

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I. Introduction

The accurate estimation of the range and damage distribution of primary knockon atoms or injected ions in materials is critical to the successful interpretation of radiation effects in nuclear reactors. Recent measurements of the ranges and damage of ions in material show that there are large differences between theory and experiment.*

In this work, a three-dimensional Monte Carlo model, HERAD, has been developed to study the range and the damage distribution of ions injected in materials. The model incorporates the options to use a large number of nuclear and electronic stopping models. The HERAD code takes into account the presence of cavities on the range and ion distribution. The results of the HERAD model are compared to the other current computational models, and the effect of cavities on the range as well as the distribution of damage is studied. The HERAD code yields a closer agreement between experiments and theory than other computational models. The code is also shown to be less expensive to run and more versatile than present Monte Carlo codes for radiation damage calculations.

The next section of this report, Section II, describes the computational model used in HERAD. Section III describes the input of the code, and Section IV gives an example for a test case. Finally, Section V shows how to obtain the code and run it.

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* For a summary, see: H. Attaya, Ph.D. Thesis, University of Wisconsin, 1981.

II. The Computational Model

II.1 Introduction

To study the effect of the microstructure on the range and damage of implanted ions in the materials, a three-dimensional Monte Carlo code called HERAD (Heterogeneous Radiation Damage) was developed which is capable of predicting the range and the damage in homogeneous or inhomogeneous materials, e.g. materials which contain voids, precipitates or bubbles.

II.2 Assumptions

The model is based on the following assumptions:

(a) the moving particle interacts with one atom at a time, i.e. the elastic binary collision approximation is assumed;

(b) the target is assumed amorphous, i.e. we neglect any periodic lattice effects;

(c) the moving particle loses energy to electrons continuously while it travels between successive collisions;

(d) the magic formula of Lindhard[1] is used to evaluate the scattering angle;

(e) the steps between successive collisions are assumed to be exponentially distributed (see Eq. 35), i.e. the mean free path assumption is taken;

(f) the moving particle is assumed to be stopped when its energy falls below a cutoff energy (~ 25 eV).

II.3 Calculation Procedure

II.3.1 Nuclear Energy Loss in a Scattering Event

The universal differential scattering cross section given by Lindhard et al.[1] is

$$d\sigma = \frac{1}{2}\pi a^2 \, t^{-3/2} \, f(t^{1/2}) \, dt \quad , \tag{1}$$

where a is the screening length given by

$$a = 0.8853\, a_o \frac{k}{g(Z_1,Z_2)} \quad . \tag{2}$$

a_o is the Bohr radius = $.529 \times 10^{-8}$ cm, and $g(Z_1,Z_2)$ is obtained either from Lindhard's formula

$$g(Z_1,Z_2) = (Z_1^{2/3} + Z_2^{2/3})^{1/2} \quad , \tag{3}$$

or from Firsov's formula

$$g(Z_1,Z_2) = (Z_1^{1/2} + Z_1^{1/2})^{2/3} \quad . \tag{4}$$

The factor k in Eq. (2) is introduced to study the effect of the screening length on the calculation results. $t^{1/2}$ is given by $t^{1/2} = \varepsilon \sin \theta/2$, where θ is the CM scattering angle, ε is the reduced energy

$$\varepsilon = E \frac{M_2}{M_1 + M_2} \frac{a}{Z_1 Z_2 e^2} \quad , \tag{5}$$

M_1 and Z_1 are the mass and the atomic number of the moving particle, M_2 and Z_2 are the mass and the atomic number of the target atom, E is the energy of the moving particle and e is the electronic charge. $f(t^{1/2})$ is given by Winterbon[2] as

$$f(t^{1/2}) = \lambda t^{1/2-m} [1 + (2\lambda t^{1-m})^q]^{-1/q} \quad , \tag{6}$$

which is valid for $0.001 < t^{1/2} < 10$, and approaches a simple analytical form

$$f_L(t^{1/2}) = \lambda t^{1/2-m} \quad , \tag{7}$$

for small values of $t^{1/2}$. For large values of $t^{1/2}$ ($t^{1/2} > 10$), we use the expression

$$f_U(t^{1/2}) = 0.5\ t^{-1/2} \quad , \tag{8}$$

which corresponds to Rutherford scattering.[3] The three different regions for $f(t^{1/2})$ are shown in Fig. 1 for the Thomas-Fermi and Moliere potentials. For very low energies where the screening effect is excessive, we use the Born-Mayer potential. The function $f(t^{1/2})$ of the Born-Mayer potential is given by Sigmund[4] as

$$f_{BM}(t^{1/2}) = 24t^{1/2} \quad . \tag{9}$$

The differential cross section is given by

$$d\sigma = (\pi a_{BM}^2)\ \frac{(24t^{1/2})}{2t^{3/2}}\ dt \quad , \tag{10}$$

where a_{BM} equals 0.219 Å. Sigmund[4] estimated a limiting energy E_{BM} given by

$$E_{BM} = k_{BM}\ [0.0234\ \frac{M_1 + M_2}{M_2}\ (\frac{a_{12}}{a_{BM}})^3 \cdot \frac{Z_1 Z_2 e^2}{a_{12}}\ ] \quad , \tag{11}$$

below which Eq. (10) can be used. a_{12} is the screening length for the

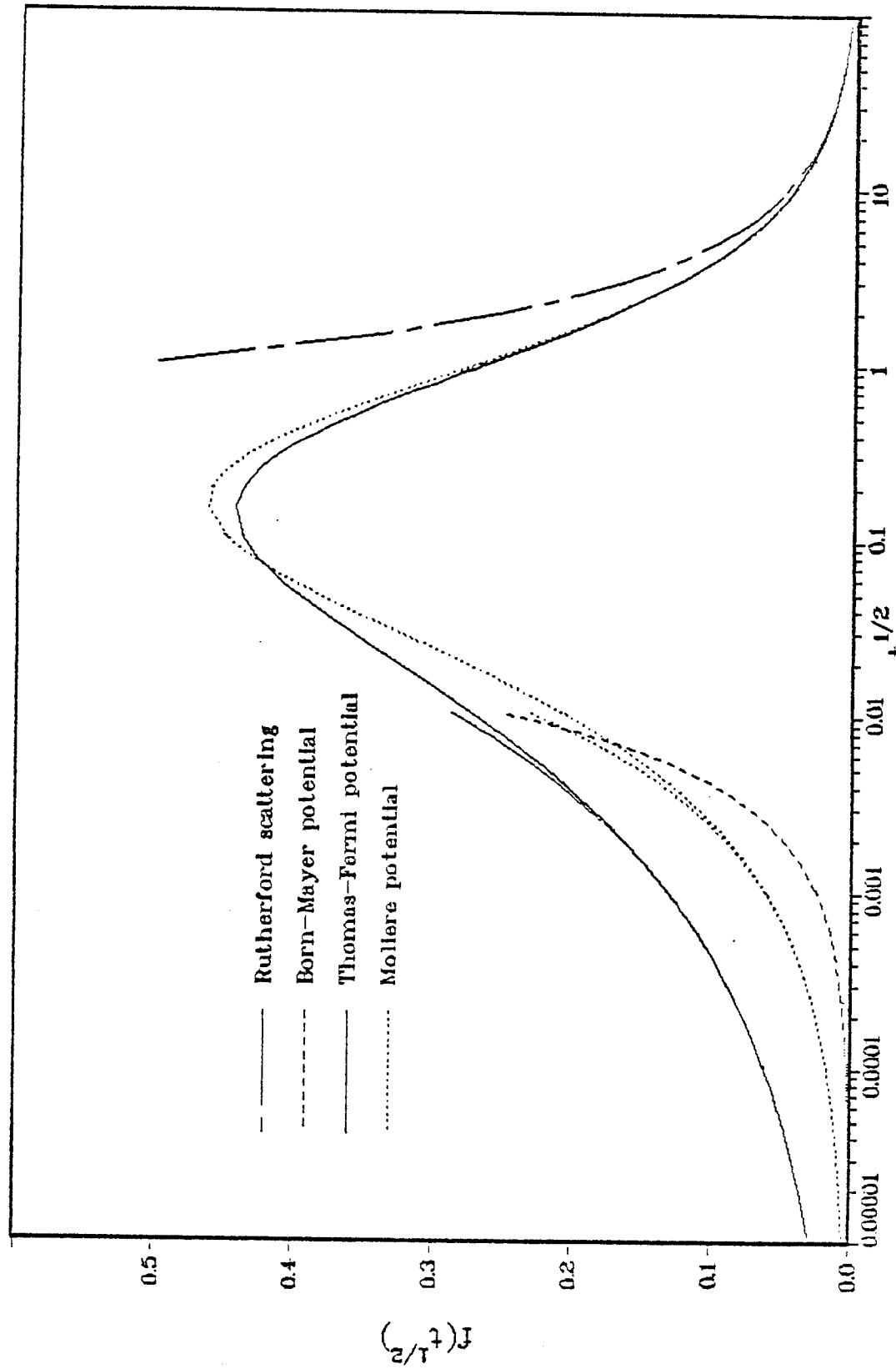

Figure 1 The universal scattering function for Thomas-Fermi, Moliere, and Born-Mayer potentials.

colliding atoms given by Eq. (2) and we introduce the factor k_{BM} to allow for the change of E_{BM}. Alternatively, E_{BM} can be assigned an input value.

Another choice for very low energy scattering is assuming isotropic scattering in the CM[5] system with

$$d\sigma = \frac{\sigma_g}{2} \sin\theta \, d\theta \quad , \tag{12}$$

where σ_g is the total effective cross section given by

$$\sigma_g = \pi P_c^2 \quad , \tag{13}$$

where $2P_c$ is the average distance between the target atoms.

The total scattering cross section is given by

$$\sigma_T = \int_{t_{min}^{1/2}}^{t_{max}^{1/2}} d\sigma \quad , \tag{14}$$

where $d\sigma$ is given by either Eq. (1) together with Eqs. (6), (7), and (8), Eq. (10), or Eq. (12), depending on the energy of the particle, the choice of the potential and the value of $t_{min}^{1/2}$,

$t_{min}^{1/2} = \varepsilon \sin(\theta_{min}/2)$,

$t_{max}^{1/2} = \varepsilon$,

and θ_{min} is the minimum angle of scattering which can be calculated from Eqs. (A.6)-(A.9), or assigned a constant value ($\sim 2°$).

The scattering angle is determined from the expression

$$\int_{t_{min}^{1/2}}^{t^{1/2}} d\sigma/\sigma_T = \rho \quad , \tag{15}$$

where ρ is a random number uniformly distributed from 0 to 1. The actual value of the scattering angle, θ, is then evaluated from the value of $t^{1/2}$ which satisfies Eq. (15) via

$$\theta = 2 \sin^{-1} \left(\frac{t^{1/2}}{\varepsilon}\right) \quad . \tag{16}$$

The nuclear energy loss is given by

$$\Delta T = \gamma E \sin^2 \frac{\theta}{2} \quad , \tag{17}$$

where $\gamma = 4M_1M_2/(M_1 + M_2)^2$, and E is the energy of the particle before collision.

The polar scattering angle of the scattered particle in the laboratory, ψ_1, can be obtained from the familiar relation

$$\tan \psi_1 = \frac{A \sin \theta}{(1 + A \cos \theta)} \quad , \tag{18}$$

where $A = M_2/M_1$. The corresponding angle of the struck particle is

$$\psi_2 = \frac{\pi}{2} - \frac{\theta}{2} \quad . \tag{19}$$

Since the scattering in the azimuthal plane is isotropic, the azimuthal scattering angle θ is uniformly distributed from 0 to π, and is determined from

$$\phi = 2\pi\rho \quad , \tag{20}$$

where ρ is another random number.

The directions of the scattered particle and the target atom (the scatterer) after any collision can be determined from the above quantites as described below. Consider that the particle moves along the vector $\bar{H}$ (see Fig. 2) before the collision and has direction cosines a_1, b_1, and c_1. If no scattering event occurs, the particle will continue to move along $\bar{H}$. Suppose that the particle at any point P along $\bar{H}$ suffers a collision which results in a deflection of its path with respect to $\bar{H}$ by the angle ψ_1 given by Eq. (18), and suppose that the particle continues to travel a unit length S. The end point of S, due to the fact that the scattering can happen in any plane containing H, may be at any point along the perimeter of the base of a cone whose altitude is the extension of $\bar{H}$.

The altitude of the cone L and its base radius will be

$$L = \cos \psi_1 \quad ,$$

and

$$R = \sin \psi_1 \quad , \tag{21}$$

respectively. The coordinates of the center of the cone base x_o, y_o, and z_o with respect to the point of collision P are given by

$$\begin{aligned} x_o &= L \cdot a_1 \quad , \\ y_o &= L \cdot b_1 \quad , \\ z_o &= L \cdot c_1 \quad . \end{aligned} \tag{22}$$

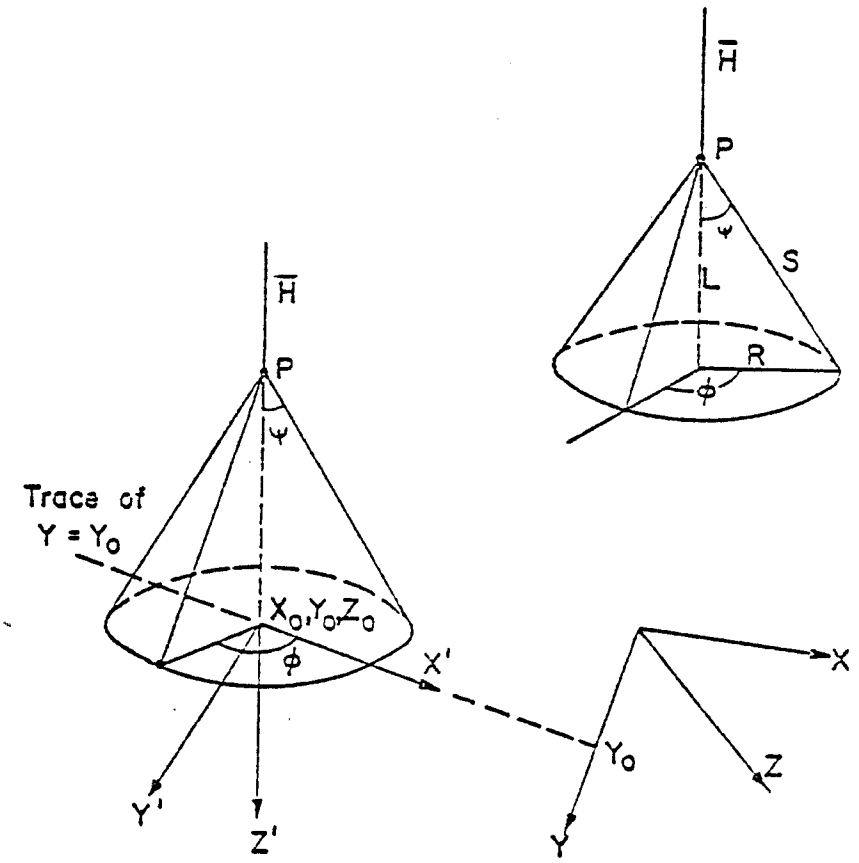

Figure 2 Coordinate systems used to locate the point of collision.

A new coordinate system is used with axes X', Y', Z' chosen such that the X'Y' plane contains the base of the cone, and Z' coincides with $\bar{H}$, i.e.

$$a_{Z'} = a_1 \quad , \quad b_{Z'} = b_1 \quad , \quad \text{and} \quad c_{Z'} = c_1 \quad . \tag{23}$$

Since the X' axis is arbitrary, it is chosen to be the line of the intersection of the plane of the base with the plane $Y = y_o$. The equation of the cone base in terms of the direction cosines of the normal to it ($\bar{H}$), and a point in the plane (x_o, y_o, z_o) is then

$$a_1 x + b_1 y + c_1 z - (a_1 x_o + b_1 y_o + c_1 z_o) = 0 \quad . \tag{24}$$

Note that the collision point P is considered as the origin of the original coordinate system XYZ. The line of intersection of the base with the plane $Y = y_o$ is

$$a_1 x + c_1 z - (a_1 x_o + c_1 z_o) = 0 \quad , \tag{25}$$

which leads to an equation for the line of the intersection (X'), given by

$$z = \left(-\frac{a_1}{c_1}\right) x + \left(\frac{a_1}{c_1}\right) x_o + Z \quad . \tag{26}$$

Therefore, the direction cosines of the X' axis with respect to the original axes are

$$a_{X'} = \cos\,(\arctan\,(-a_1/c_1)) \quad ,$$

$$b_{X'} = \cos\,(\pi/2) = 0 \quad , \tag{27}$$

$$\text{and} \quad c_{X'} = \cos\,(\arctan\,(-c_1/a_1)) \quad .$$

The direction cosines of the Y' axis, knowing that of X' and Z' are

$$a_{Y'} = b_{Z'}c_{X'} \quad ,$$

$$b_{Y'} = c_{Z'}a_{X'} - c_{X'}a_{Z'} \quad , \tag{28}$$

$$c_{Y'} = -a_{X'}b_{Z'} \quad .$$

The azimuthal angle ϕ is chosen with respect to the X' axis by Eq. (20). Then the coordinates of the point N (Fig. 2) in the X'Y'Z' system are

$$x'_N = R\cos\,\phi$$

$$y'_N = R\sin\,\phi \tag{29}$$

$$z'_N = 0 \quad ,$$

which can be transformed back to the original system XYZ, whose origin is the point P, to give

$$x_N = a_{X'}x'_N + a_{Y'}y'_N + x_o \quad ,$$

$$y_N = b_{X'}x'_N + a_{Y'}y'_N + y_o \quad , \tag{30}$$

$$z_N = c_{X'}x'_N + a_{Y'}y'_N + z_o \quad .$$

Finally the new direction cosines of the scattered particle are

$$a_n = x_n/D \quad , \quad b_n = y_n/D \quad , \quad c_n = z_n/D \quad , \tag{31}$$

where

$$D = (x_N^2 + Y_N^2 + Z_N^2)^{1/2} \quad . \tag{32}$$

The direction cosines of the scatterer are obtained by solving the vector equations

$$\begin{aligned} \bar{s} \cdot \bar{P}_1 &= \cos \psi_2 \quad , \\ \bar{s} \cdot \bar{P}_2 &= \cos (\psi_1 + \psi_2) \quad , \\ \text{and} \quad (\bar{P}_1 \times \bar{P}_2) \cdot \bar{s} &= 0 \quad , \end{aligned} \tag{33}$$

where $\bar{P}_1$ is a unit vector in the direction of the moving particle before collision, $\bar{P}_2$ is a unit vector in the direction of the particle after collision, $\bar{s}$ is a unit vector in the direction of the displaced atom, ψ_1 is the laboratory scattering angle given by Eq. (18), and ψ_2 is the laboratory scattering angle of the scatterer and is given by Eq. (19). Figure 3 shows the directional relations among the three vectors.

Equation (33) can be put in the following form

$$\begin{aligned} a_s a_1 + b_s b_1 + c_s c_1 &= \cos \psi_1 \\ a_s a_2 + b_s b_2 + c_s c_2 &= \cos(\psi_1 + \psi_2) \\ a_s(b_1 c_2 - c_1 b_2) + b_s(c_1 a_2 - a_1 c_2) + c_s(a_1 b_2 - b_1 a_2) &= 0 \end{aligned} \tag{34}$$

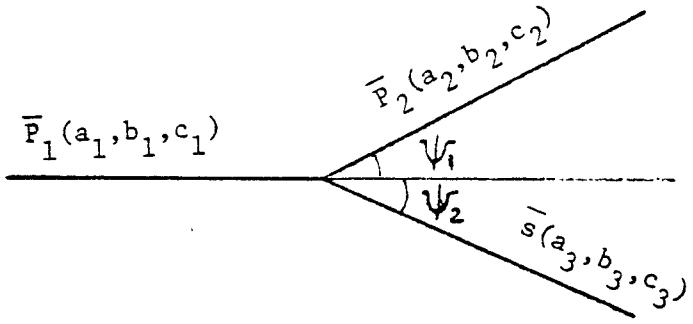

Figure 3 Schematic diagram showing the directions of the moving particle before collison $\overline{P}_1$, after collsion $\overline{P}_2$ and the direction of the recoil atom s.

where (a_1,b_1,c_1) are the direction cosines of $\bar{P}_1$, (a_2,b_2,c_2) are the direction cosines of $\bar{P}_2$, and (a_3,b_3,c_3) are the direction cosines of $\bar{s}$.

II.3.2 Step Length Between Two Successive Collisions and the Electronic Energy Loss

The step length, ℓ, between two successive nuclear collisions is assumed to be exponentially distributed, i.e.

$$p(\ell) = \frac{1}{\sigma_T N} \exp\left(-\frac{\ell}{\sigma_T N}\right) \quad , \tag{35}$$

where N is the atomic density of the target, and σ_T is the total scattering cross section which is obtained from Eq. (14). The value of ℓ is then evaluated from

$$\ell = -\frac{1}{N\sigma_T} \ln(\rho) \quad , \tag{36}$$

where ρ is a random number uniformly distributed between 0 and 1.0.

A truncated exponential distribution, which limits the minimum step and/or the maximum step, can also be used. Another constraint on the step length is made such that the electronic energy loss of the particle along the step does not exceed some fraction (~ 5%) of the energy of the particle at the beginning of the step. Such a constraint was also used by Biersack.[6]

The electronic energy loss is assumed to be continuous along the path of the particle. If the step length is ℓ and the energy of the particle is E_i at the beginning of the step, then the energy of the particle, E_f, at the end of the step ℓ is given by

$$E_f = E_i - \int_0^{\ell} \left(\frac{dE}{d\ell}\right)_e d\ell \quad , \tag{37}$$

and for the first order approximation one gets

$$E_f = E_i - \left(\frac{dE}{d\ell}\right)_e (E_i)\ell \quad . \tag{38}$$

The Lindhard[7] or Firsov[8] formulas, can be used for $(dE/d\ell)_e = S_e N$, where N is the atomic density. The LSS formula for S_e is given by

$$S_e = 8\pi e^2 a_o \xi_e (Z_1 Z_2 / Z) v / v_o \quad , \tag{39}$$

where $$Z^{2/3} = Z_1^{2/3} + Z_2^{2/3} \quad ,$$

and $$\xi_e \approx Z_1^{1/6} \quad ,$$

and the Firsov formula is

$$S_e = 7.51(3\pi^2 \hbar a_o/32)(Z_1 + Z_2)v_1 \quad . \tag{40}$$

The Brice[9] formula for S_e can be used also, and is given by

$$S_e = A(Z_1 + Z_2) f_b(U) \left[U^{1/2} \left(\frac{(30U^2 + 53U + 21)}{(3 + 3U^2)}\right) + (10U + 1)\arctan(U^{1/2})\right] \quad , \tag{41}$$

where: $A = 0.60961 \times 10^{-15}$ eV cm^2/atom,

$U = E/(Z^2 M_1 E_1)$,

$E_1 = 99.20$ KeV

$$f_b(U) = [1 + (4Z^2\ a'^2\ U)^{n/2}]^{-1},$$

and Z, a', and n are the three parameters for projectile target combination.

II.3.3 The Displacement Model

The computer program HERAD is designed to study the range distribution as well as the damage distribution of ions in materials. In the first case, only the incident ions are followed. An approximate estimate of the damage energy, i.e. the amount of energy that results in displacement and defect production, can be made. If ΔT is the energy loss by the incident ion upon a collision with a target atom, E_d is the threshold energy of the displacement, and ΔT is less than E_d, ΔT is assumed to be dissipated into phonons, i.e. heat. If ΔT is greater than E_d, ΔT is partitioned according to Lindhard[10] to a damage energy T_D which ultimately goes to displacement and electronic energy T_e which is lost to electrons. T_D and T_e are given by

$$T_D = \Delta T/(1 + kg(x)) \quad ,$$

and (42)

$$T_e = \Delta T - T_D \quad ,$$

where

$$k = (0.1334\ Z_2^{2/3})/A_2^{1/2} \quad , \tag{43}$$

$$x = \Delta T/(0.02693\ Z_2^{7/3}) \quad , \tag{44}$$

and[11]

$$g(x) = x + 0.4024\ x^{3/4} + 3.4008\ x^{1/6} \quad . \tag{45}$$

The damage energy T_D is supposed to be deposited at the point of collision, such that the spatial distribution of T_D will not include the recoil effect. The number of defects, ν, according to the Kinchin and Pease displacement

model[12] is

$$\nu = \frac{T_D}{2E_d} \quad , \tag{46}$$

which is based on the hard sphere potential. For more realistic potentials, Eq. (46) becomes[11]

$$\nu = \eta \frac{T_D}{2E_d} \quad , \tag{47}$$

where η (~ 80%) is the displacement efficiency which is a function of the interatomic potential.

A more precise estimate of the damage can be made by following the primary knock atoms. In this case, T_D given by Eq. (42) is deposited at the end of the PKA trajectory when its energy is less than $2E_d$, i.e. no longer able to produce further displacements. Finally, the defect distribution can be estimated by following every atom in the cascade capable of displacing a target atom. Figure 4 shows and explains the displacement model adopted in the calculations. The cutoff energy E_c may be either E_d or $2E_d$ and in both cases a binding energy U_{bin} may be optionally included to account for the amount of energy the recoil atom may expend in breaking its bonds in the lattice. The value of the cutoff energy E_c can also take any pre-assigned value which allows us to compare our results with other calculations that employ different values for E_c, E_d, and U_{bin}.

II.4 Inhomogeneous Target

In dealing with an inhomogeneous material, i.e. a material containing voids or bubbles, we assume that the cavities are randomly distributed in the

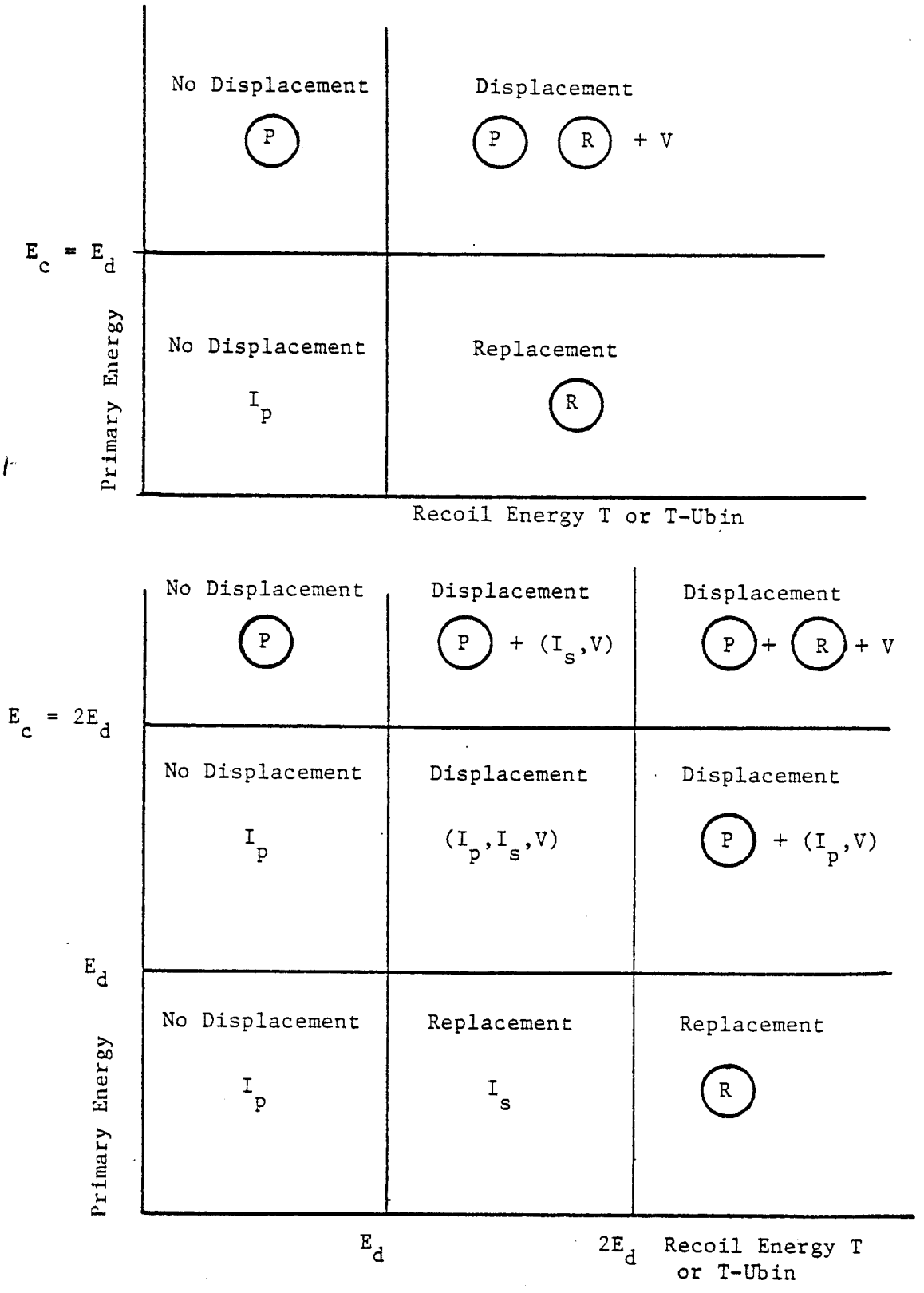

Figure 4 a) The displacement model when the cutoff energy = E_d; b) when the cutoff energy = $2E_d$; P=primary, R=recoil, I_p=interstitial results from a primary, I_s=interstitial results from a secondary; ( )=near defect, ◯ =energetic particle to be followed.

material with known distributions of the number density and the average diameter, or the distributions of the void fraction of the cavities. It is known[14-16] that

$$V_V = L_L \quad , \tag{48}$$

where V_V is the volume fraction of the second phase, and L_L is the lineal fraction, i.e. the length of lineal intercepts per unit length of a random test line.

This fact has been used by Odette et al.[17] to estimate the effect of voids on the range and damage of ions in materials, but in that work no difference was made between the path of the ion and its projected range. In our calculations the steps between collisions, Eq. (36), were increased according to Eq. (48) by

$$\Delta\ell = \ell \cdot V_V \quad , \tag{49}$$

and the particle energy remains the same as it transverses the void. Thus, in this model the actual path of the moving particles will be affected by the presence of the cavities, rather than the projected range as in the model of Odette et al.[17]

II.5 The Computer Code HERAD

Figure 5 shows a block diagram of the computer program HERAD. The name "HERAD" stands for "Heterogeneous Radiation Damage". The following is a brief description of the code and the function of the procedures used in it.

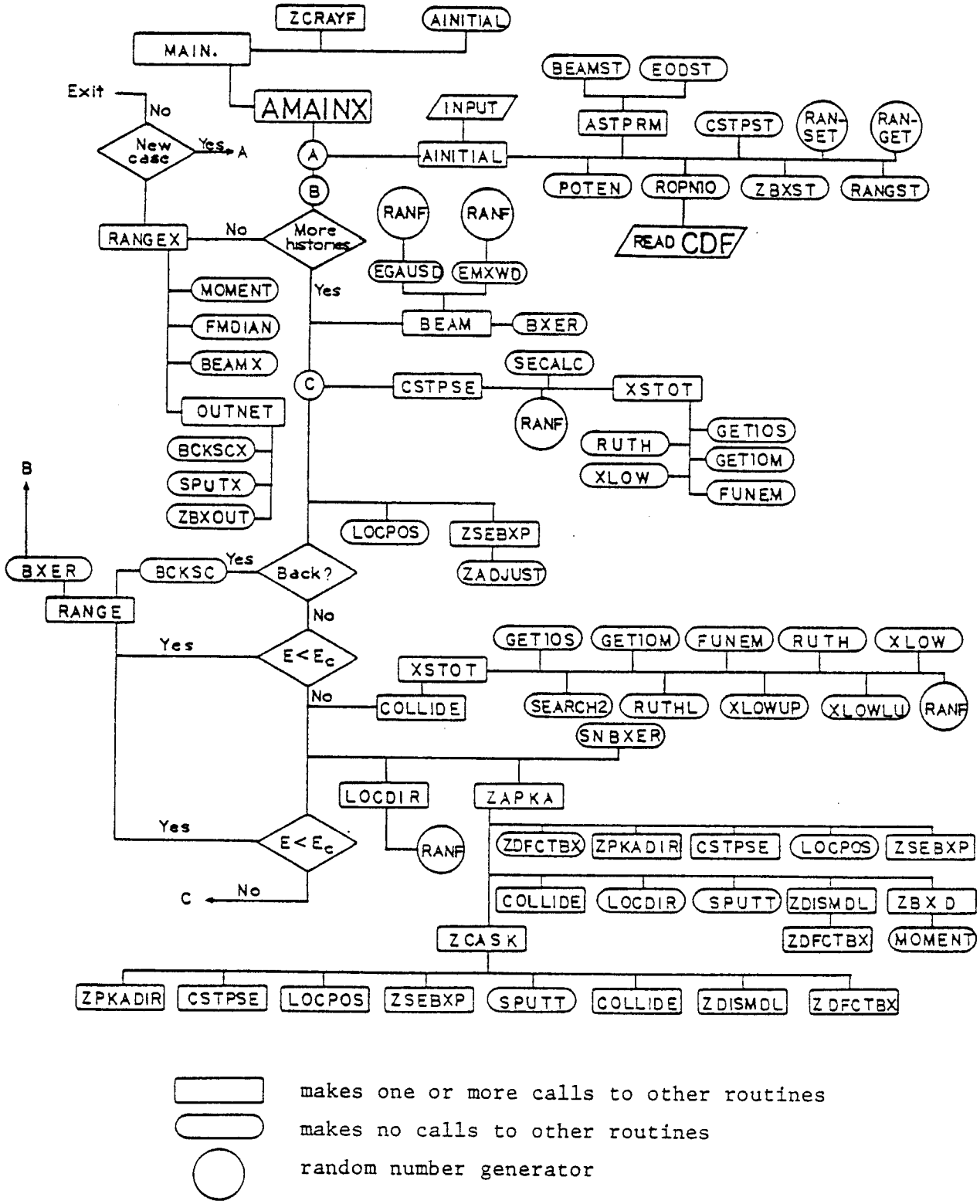

Figure 5 Flow Diagram for HERAD.

MAIN. MAIN is the starting procedure. It calls ZCRAYF, AINITIAL, and AMAINX.

ZCRAYF. ZCRAYF handles the input/output files according to the computer environment, i.e. if the program is to be run on a CRAY-1 or CDC-7600 machine.

AINITIAL. This subroutine is called twice, first by MAIN to set the physical constants needed in the calculations, and second by AMAINX to set some of the input data to their default values and read the input data. AINITIAL calls POTEN, ROPN1Ø, ZBXST, ASTPRM, and CSTST.

AMAINX. This is the main controller of the program. AMAINX follows the incident ions only, and it calls ZAPKA to follow the PKAs if that is requested.

POTEN. POTEN is used to set the potential constants, used in the calculation of the cross section, λ, m, and q in Eq. (6).

ROPN1Ø. ROPN1Ø is an entry point in the subroutine ENTRYS, and is called to read the CDF of the potential which resides in an input file produced by the program POTSET.

ASTPRM. ASTPRM calculates most of the parameters and constants used in other procedures. Also, it calls the setting entry points BEAMST and EODST.

BEAM. BEAM provides the energy of the incident beam of ions. Three different distributions may be used for the incident beam, mono-energetic, Gaussian, or Maxwellian. In the case of the Gaussian distribution the function EGAUSD is used, and in the case of a Maxwellian distribution the function EMXWD is used. In both cases a call to BXER is made to record the energy.

EGAUSD. The function EGAUSD uses the Monte Carlo method to sample a Gaussian distribution knowing its mean and its standard deviation. The method employed is known as the sine-cosine method.[18,19]

EMXWD. This function also uses the Monte Carlo method to sample a Maxwellian distribution.[18]

BXER. BXER is used to record a variable into its associated histogram.

CSTPSE. This procedure outputs the step length between two collisions and the electronic energy loss of the particle along this step. It calls XSTOT, the random number generator RANF, and in case that the Brice formula is used for the electronic energy loss it calls SECALC.

SECALC. SECALC calculates the electronic energy loss according to the Brice formula (Eq. 41).

XSTOT. XSTOT calculates the total scattering cross section and the scattering angle.

LOCIR, LOCPOS. LOCDIR determines the direction cosines of the scattered particle after scattering knowing the angle of scattering. LOCPOS determines the coordinates of the next collision of the particle giving the step length and the direction cosines.

ZSEBXP. ZSEBXP is used to record the electronic energy loss in a histogram.

COLLIDE. Calculates the laboratory scattering angle and the nuclear energy loss in the collision.

ZAPKA. This routine follows the PKAs if requested.

SNBXR. Records the nuclear energy loss of the incident ions in the collisions with respect to the space.

BCKSC. Records the energy of the backscattered particles.

DEEFF. Calculates the partition of the PKA energy into electronic and nuclear energy according to Lindhard, Eqs. (42)-(44).

ENTRYS. It has the entry points, ROPN1Ø which was mentioned before, GETIOS, and GETIOM. GETIOS and GETIOM return the values of CDF and the PDF of the scattering cross section.

SPUTT. Calculates the energy distribution of sputtered atoms.

EMEDIAN. Returns the median of a distribution.

FUNEM. Calculates the minimum angle of scattering.

MOMENT. Calculates the average, the standard deviation, the skewness, and the kortosis of a distribution.

RANGE. Calculates the vector range, the projected range, the spread, and the total path at the end of a history and calls BXER to record all the above quantities in their histograms. At the end of all histories the energy points, RANGEX is called to print out these histograms, to call MOMENT, and to print the statistics.

RUTH, XLOW. Calculates the upper and the lower limit of the scattering function, respectively.

SEARCH2. Searches for the value of $t^{1/2}$ which satisfies Eq. (15).

ZADJUST. Is called by any scoring routine when the score is out of the limit of the histogram; it then doubles the histogram interval and adjusts the scores in the histogram.

ZBXD. Calculates the distribution of the damage energy transported by the PKAs and the statistics of this distribution.

ZCASK. This routine is called from ZAPKA if all the displaced atoms are to be followed. It follows a displaced atom by a PKA. During the slowing down of this atom, the secondary, ZCASK stores the coordinates, the direction cosines, and the energy of any displaced atom capable of producing more displacements. After the energy of the moving atom falls below the cutoff

energy, ZCASK retrieves the latest stored coordinates, directions, and energy and starts another branch in the cascade. This is done until all the stored information is processed.

ZDISMDL. This routine is called by ZAPKA and ZCASK. It employs the displacement model in the collisions and scores the resulting defects by calling ZDFCTBX.

ZPKADIR. Calculates the direction of a recoil atom in a collision.

OUTNET. This is the main output routine. It calculates and prints out a complete energy partition, different energy distribution, collision distribution, and defect distributions. If plotting is requested, OUTNET writes the desired information on an output file to be processed by the plotting programs.

HERAD can be compiled to include graphic routines which help one to watch the paths of the moving particles, projected on any plane, on a display terminal. This was mainly used as a debugging tool instead of having a huge amount of print output describing the trajectories of the particles at each collision. An example of this output is shown in Fig. 6.

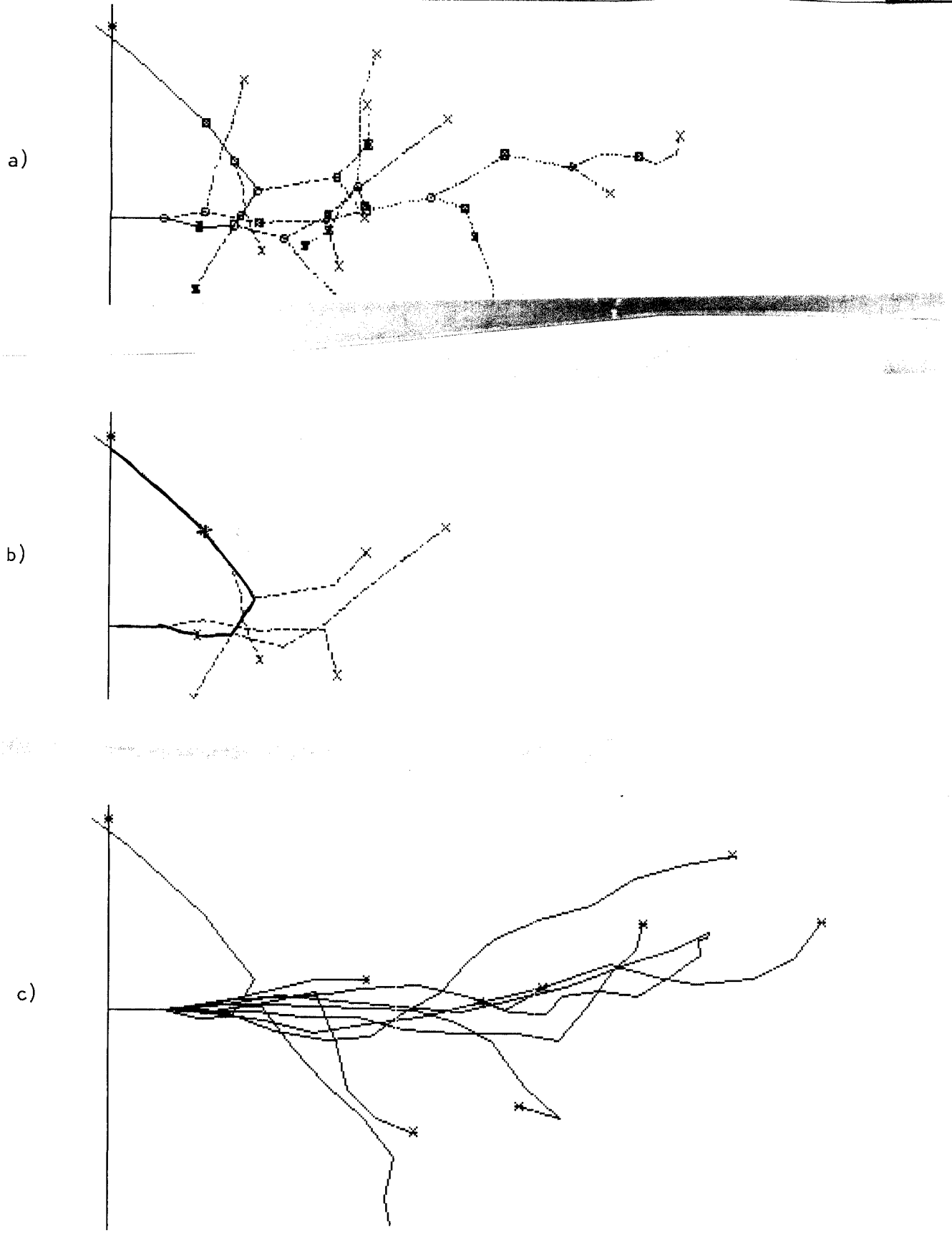

Figure 6 Display output from HERAD: a) 10 histories of 2 keV Cu-Ni; b) trajectories of PKAs produced by one history of 2 keV Cu ion on Ni; c) the complete cascade developed by one history of 2 keV Cu ion in Ni.

III. Input Description

III.1 Introduction

The input to the HERAD code is simple. Only two records are required: a title card at the beginning, then a namelist record which sets the values of some or all of the input variables. There is an optional control card which contains either the word "NEW" to start a new case, or the word "END" to terminate the program.

The file which contains these input records, after being read for the first time by the program, would have an additional record at its beginning. The record is an integer number of ..ØØ in I3 FORMAT. All the output files will be named using this number. The number will be incremented by 1 every time the file is read by HERAD. See Section V.3 for the naming convention used by HERAD. In the following is a description of each record.

III.2 Title Card

This record contains up to 8Ø ASCII characters used as a title to the problem and will appear on the top of every output section. If no title is required, this record should be left blank. An important restriction on this record is that the first three characters of this card should not contain any integer number.

III.3 First Namelist Input Record

ALAT. Default (none): is the cube root of the volume of the unit cell of the target materials. Note only mono-component targets are allowed in this version of HERAD. ALAT together with NFORM are used to calculate the atomic density of the target (see ALATA and ALATD for other alternatives).

NFORM. Default (Ø): this is the number of atoms in the unit cell (used only if ALAT is used).

ALATD. Default (Ø.Ø): the gram density (gm/cm^3) of the target, and is an alternative to ALAT and ALATA.

ALATA. Default (Ø.Ø): the atomic density (atoms/cm^3) of the target, and is an alternative to ALAT and ALATD. Note: only one of the three variables (ALAT, ALATD, and ALATA) should be used, and the other two should be set to zeros.

PT. Default (Ø.Ø): the atomic mass (amu) of the target atoms.

ZT. Default (Ø.Ø): the atomic number of the target atoms.

ED. Default (25.): the average displacement energy of the target atoms in eV.

PI. Default (Ø.Ø): the atomic mass (amu) of the incident ion.

ZI. Default (Ø.Ø): the atomic number of the incident ion.

EION. Default (Ø.Ø): the energy of the incident ions in keV.

EDIM. Default (25.): the cutoff energy of the incident ion, i.e. an ion's history is ended when ion's energy has a value ≤ EDIM.

ACI. Default (Ø.Ø): the direction cosine of the angle between the incident direction of the ion and the x-axis.

BCI. Default (Ø.Ø): the direction cosine of the angle between the incident direction of the ion and the y-axis.

CCI. Default (1.): the direction cosine of the angle between the incident direction of the ion and the z-axis.

XOO. Default (Ø.Ø):
YOO. Default (Ø.Ø):
ZOO. Default (Ø.Ø):

} the cartesian coordinates of the point of ion injection (it could be inside the target)

LMONO. Default (.TRUE.): to use monoenergetic beam.

LGAUS. Default (.FALSE.): if set to .TRUE. the program will sample Gaussian energy distribution for the incident beam with EION as the average energy of the distribution and ESIGMA as its standard deviation.

ESIGMA. Default (Ø.Ø): the standard deviation of the Gaussian energy distribution (in keV) of the beam and used if LGAUS is set to .TRUE. .

LMAXW. Default (.FALSE.): if a Maxwellian energy distribution of the incident beam is required this variable should be set to .TRUE. and the variable EKT should be set to the maximum energy (in keV) of the distribution.

EKT. Default (Ø.Ø): see above.

SEFRM(1). Default ("LSS"): this variable sets the electronic energy law used for the incident ion in the target. Other choices are: "FIRSOV", "BRICE", and "EXPR". If SEFRM(1) = "BRICE", the user should supply the three parameters for Brice formula,[9] which uses SETA(1), ALP(1), and EN(1) (see below). If SEFRM = "EXPR", the user should include in the input the values of NEXP(1) and CSE(1) (see below).

SEFRM(2). Default ("LSS"): exactly as SEFRM(1), but is used to set the electronic energy law which governs the electronic energy loss for the recoils (i.e., the target atoms) in the target.

SETA(1). ALP(1). EN(1). } The three parameters Z, A, and N of the Brice formula for the ion-target electronic interaction.

SETA(2). ALP(2). EN(2). } As above, but for target-target electronic interaction.

NEXP(1), CSE(1). If SEFRM(1)="EXPR" the program will use the following formula for the electronic energy loss

$$S_e/N = CSE(1)E^{(NEXPC1/1ØØ)}$$

where E is the energy in keV, N is the target atomic density (atom/cm^3), and S_e is the electronic stopping power for the incident ions in the target. S_e/N should be in the units of $1Ø^{-18}$ keV-cm^2/atom.

NEXP(2), CSE(2). As above but for the recoils in the target.

CKL(1). Default (1.): a coefficient which can be used to decrease (or increase) the electronic stopping power of the ion.

CKL(2). Default (1.): as above but for the recoils.

SELIMT. Default (5.): this is to impose a constraint on the length of the step between two successive collisions such that the electronic energy loss along that step should not be greater than (SELIMT/1ØØ.)E, where E is the energy of the particle at the beginning of the step. To remove this constraint SELIMIT should be set to any negative value.

SMIN. Default (1.): this is another constraint on the step between collisions. The value of SMIN is in the unit of the average distance between the target atoms, and it sets minimum distance the particle can take between collisions. To remove this constraint set SMIN to any negative value.

SMAX. Default (1ØØ.): also in units of the average distance between the target atoms, it sets the maximum distance a moving particle can take between two successive collisions.

POT & FILENAME. POT is the name of the potential used to describe the nuclear interaction, and FILENAME is the name of the file which contains the cumulative distribution function of that potential. There are six potentials available; the following table gives the default file name for each one.

POT	FILENAME	Potential
tf	ptfe4	Thomas-Fermi
tfs	ptfse4	Thomas-Fermi-Sommerf
bohr	pbohre4	Bohr
lz	pLze4	Lenz-Jensen
mol	pmole4	Moliere
tfb	ptfbe4	Thomas-Fermi as was suggested by Biersack[23]

The cumulative distribution function for any of these potentials is calculated and written by the program XPOTEN which will be described briefly in the next chapter.

ANGLI(I), I=1,2. Default (1.,1.): the cutoff angle (in degrees) for calculating the collision cross section for ions (I=1) and recoil (I=2). Alternatively one can set this lower limit in terms of energy (see LANG and EM).

LANG(I), I=1,2. Default (.FALSE.,.FALSE.): if LANG(I)=.TRUE. the program will use the value of EM(I) as the lower limit in evaluating the collision cross section integrals.

EM(I), I=1,2. Default (=ED): energy in eV for the lower limit of the integration of the cross section.

UBIN. Default (Ø.Ø): the binding energy of the target atoms in eV.

UF. Default (2.ED): a cutoff energy in eV used together with ED to control the displacement model (see Fig. 4).

CESTR(I), I=1,2. Default (1.): this is the coefficient k_{BM} used in Eq. 11 to allow for changing the value of the energy below which the cross section is calculated using Eq. 5.

LFRSV. Default (.FALSE.): if LFRSV=.TRUE. the program uses the screening length of Firsov given by Eq. 4 instead of using Lindhard's value (the default).

CSCRN(I), I=1,2. Default (1.,1.): the factor k in Eq. 2.

LPRIM(1). Default (.FALSE.): if LPRIM(1)=.TRUE., the program will follow all the primary knockon atoms generated in the collisions of the incident ion with target atoms.

LPRIM(2). Default (.FALSE.): if LPRIM(2)=.TRUE. the program will follow every displaced atom generated in the collisions of either the incident ions or the target recoils, i.e. a complete cascade is simulated.

LHET. Default (.FALSE.): if LHET is set to .TRUE. the program will read a second namelist input which sets the experimental void distribution function.

NHIST. Default (none): the number of histories (incident ions).

ISTP. Default (=NHIST): if ISTP is set to a value less than NHIST the program will output the statistical results every ISTP histories.

ISEED. Default (Ø on the CRAY computers, ØØ7777772ØØØØØ1B on the CDC76ØØ computer), the seed of the random number generator.

NORM. Default (1): the statistical outputs are normalized to "NORM" value.

BXV. Default (5Ø. angstroms): the initial value of the channel incident ions.

BXD. Default (5Ø. angstroms): as BXV but for the incident ions depth histogram.

BXP. Default (5Ø. angstroms): as BXV but for the incident ions path length histogram.

BXR. Default (5Ø. angstroms): as BXV but for the perpendicular range histogram.

BXE. Default (5Ø. angstroms): the initial value of the channel width of the histogram used to tail all energy quantities as well as displacements, replacements, etc.

INTORM(I): This logical array is used to control the outputs of the program. The different elements have the following effects:

I=1. Default (.FALSE.): if .TRUE. outputs the coordinates and the energy of the incident ions every collision.

I=2. Default (.FALSE.): as INFORM(1), but for the PKAs.

I=3. Default (.FALSE.): as INFORM(1), but for secondaries.

I=4. Default (.FALSE.): if .TRUE. outputs the coordinates and the energy of the incident ion at the end of each history.

I=5, I=6. Default (.TRUE.,.TRUE.): to control the output of histograms every "ISTP" histories. To get that output only after "NHIST" set INFORM(5)=.FALSE. and INFORM(6)=.TRUE. . To suppress the output of this part set both .FALSE.

I=7. Default (.TRUE.): to calculate and output the energy balance of ions.

I=8. Default (.TRUE.): to calculate and output energy balance of PKAs.

I=9. Default (.TRUE.): to output the distribution of energy deposited into damage, electronic, and the distribution of various defects.

I=1Ø. Default (.TRUE.): to output the energy distributions of the back-scattered ions and the sputtered atoms.

LPLOT. Default (.FALSE.): if LPLOT=.TRUE. the program will write its output on a binary file which will be used later by the graphic program XPLOT.

LPLTK(I), I=1,3. Default (.FALSE.,.FALSE.,.FALSE.): if the program is compiled so as to include graphic routines, the program will output to the user terminal (which should be a graphic terminal) the trajectory of the ions (if LPLTK(1)=.TRUE.), the trajectory of the PKAs (if LPLTK(2)=.TRUE.), and the trajectory of the secondaries (if LPLTK(3)=.TRUE.) (see next section on how to compile the program and using this option). Although the inclusion of the graphic routines makes the program considerably

bigger and slower, this option was a powerful tool in the debugging process of the program.

ZMINA, ZMAXA, YMAXA. Default (-5.,3ØØ.,1ØØ): sets the graphic window in the target which would be seen on the terminal's screen. ZMINA, ZMAXA set the depth range, and YMAXA sets the perpendicular range such that the left corners on the screen have the coordinates (ZMIN,$_-$YMAXA) and (ZMIN,YMAXA) with respect to the target. The right corners have the coordinates (XMAXA,$_-$YMAXA) and (ZMAXA,$_+$YMAXA).

III.4 Second Namelist Record

This is required if the logical variable "LHET" in the first namelist record above has been set to .TRUE. This namelist record has the following variables:

NOREGV. The number of intervals in the void distribution. This should not be greater than 2Ø (intervals).

VOIDBX(1). The depth coordinate of the LHS of the first interval (in angstroms).

VOIDBX(2). The interval width (in angstroms).

VOIDFR(I), I=1,2Ø. The percentage void fraction of the i-th interval.

IV. Sample Problem

A case for 901.3 keV Be ions incident on U target is presented here. The input for this case is shown below:

```
 1      be+ ions (901.3  kev)  on u target
 2   filename= "ptfe4"    , pot="tf"
 3   zt=92. ,  pt=238.1   , alata=4.725e22
 4   zi=4.    ,  pi=9.013
 5   sefrm="brice", "lss"
 6   seta(1)=2.245   alp(1)=.285      en(1)=2.943
 7   eion=901.3    , nhist=1000       , istp= 00
 8   edim=25.0  ed=25.  anali=1.0,1.0
 9   lprim=.t..,   .t..
10   lplot=.t..
11   bxv=50.     bxr=50.  bxd=50.  bxp=50.     bxe=50.
12   smin=1. , smax= 1000.   , selimt= 5. $
13   *
```

1000 histories are used and full cascade simulation is requested (LPRIM=.TRUE.,.TRUE.). The user should be cautious in using this option with such number of histories with high energies because it could be very expensive. Minimal input was used, in this case. The output for this case is given in the next pages. The first page is a list for the input.

The next page of the output shows all the parameters of this case (atomic number, etc.). Next the analysis for the incident ion range (depth, path, spread, and vector range), and histograms of the distributions of each of these quantities is shown.

After that a complete energy balance is given. Next to the energy balance there is a table which contains the distribution along the target depth of the following quantities normalized to 1 incident ion: the average number of collisions made by the ion, the electronic energy loss (ioniz.), the nuclear energy loss (nuclear), the energy of the displaced recoils (displac.), the electronic energy loss of the recoil (rec-ionz), the energy lost in non-displaced collisions (phonon), the damage energy carried by PKAs (dmg/pka), the electron energy loss by the PKAs (se/pka), the electronic energy loss by

the secondaries (se/scnd), and the distributions of the defects (V for vacancies, I for interstitials, V-I for near vacancy-interstitial pairs, and Rplc for the replacement events). Finally an energy distribution for the backscattered ions followed by the energy distribution of the sputtered atoms is given.

Graphic outputs of this case using the controllee "XPLOT" are also shown (Figs. 7-10).

```
                                                                  date     : 09/15/82
                                                                  time     : 08:05:17 (pst)
                                                                  machine  : c
controllee: xherad          controller:
loaded on : 09/14/82        at time    : 13:37:36
dropfile  : +xheradd        system     : d
user #    : 001450          account    : 862swi
program bank( min:sec ) :   19:59
pool    bank( minutes ) :         108


files:
          obeu00      qbeu00


                          ***** input data  for  run no.beu00      *****


   1 -- :  0                                                                  - herad    beu00
   2 -- :   be+ ions (901.3  kev)  on u target                                - herad    beu00
   3 -- :filename= "ptfe4"    , pot="tf"                                      - herad    beu00
   4 -- :zt=92. ,  pt=238.1  , alata=4.725e22                                 - herad    beu00
   5 -- :zi=4.   ,  pi=9.013                                                  - herad    beu00
   6 -- :sefrm="brice", "lss"                                                 - herad    beu00
   7 -- :seta(1)=2.245   alp(1)=.285     en(1)=2.943                          - herad    beu00
   8 -- :eion=901.3   , nhist=1000     , istp= 00                            - herad    beu00
   9 -- :edim=25.0  ed=25.  anqli=1.0,1.0                                     - herad    beu00
  10 -- :lprim=.t..,  .t..                                                    - herad    beu00
  11 -- :lplot=.t..                                                           - herad    beu00
  12 -- :bxv=50.    bxr=50.  bxd=50.  bxp=50.    bxe=50.                      - herad    beu00
  13 -- :smin=1. , smax= 1000.  , selimt= 5. $                                - herad    beu00
  14 -- :*                                                                    - herad    beu00
ion   potential tf     constants m,q,lamda =      0.33300     0.66700     1.30900
     the file to be accessed is ptfe4
     lamda = 1.3090  m = 0.3330  q = 0.6670
     number of intervals = 10000  minimum t1/2 =    0.00100  max. t1/2 =     10.000  index con. factor =   1000.000

ranf  iseed setting =        163287475723473
```

be+ ions (901.3 Kev) on u target

atomic density = 4.725000e+22 atom/cc
density = 18.679 gm/cc
density (input)= 0.00000 gm/cc

	ion	recoil
atomic number	4.000	92.00
atomic mass	9.013	238.1
lindhard max.energy(Kev)	1419.	2.4525e+06
e1=27.211*a*z**1.376(kev)	1.652	3263.
lindhard: (used)		
eff. charge	109.6	260.2
(z1*.67+z2**.67)**.5	4.785	6.384
screening length (cm)	9.7956e-10	7.3422e-10
firsov :		
(z1**.5+z2**.5)**.67	5.122	7.166
screening length (cm)	9.1519e-10	6.5412e-10
coeff. of epslon (1/Kev)	1.7812e-02	3.0122e-04
charact. energy(Kev)	56.14	3320.
ceoff. of rho (1/angst.)	2.0022e-04	8.0022e-04
estar (Kev)	0.1175	2.928
m2/m1	26.42	
gamma	0.1405	1.000
potential	tf	tf
coeff. for screen.	1.000	1.000
classical min vel(cm/sec)	0.7466e+05	7266.
classical min. energy(ev)	2.6032e-02	6.5134e-03
coeff. of eta(Kev)	56.14	3320.
coeff. of Kapa(sqrt(Kev))	0.1100e+05	1.3008e+06
cutoff energy(ev)	25.00	50.00
displacement ''		25.00
binding energy(ev)		0.0000
limiting angle(degree)	1.000	1.000
limiting energy(ev)	3.000	3.000
no. histories	1000	

electronic energy

	nexp	se form	cse	z	a	n	coeff.
ion	-1	brice		2.2450	0.2850	2.9430	1.00
recoil	0	lss	8.142625e-03				1.00

geometric cross section (cm**2)
max. xs = 7.651245e-16
min. step = 3.12120

	alat	averge fcc	n**(- 1/3),n**(- 2/3)	pu*ro**2 = n**(- 2/3)
min. step	0.000000	0.000000	2.76609	3.12120
geom. xst	0.000000	0.000000	7.651245e-16	7.651245e-16

incident beam : monoenergetic energy (mev) = 0.90130

: reduced energy = 16.054

1 be+ ions (901.3 kev) on u target

0 analysis of primary recoil ranges (992 particles)

	mean	median	variance	skewness	kurtosis	std dev.	error
penetration	9854.73	10243.2	0.550029e+07	-1.04462	1.21463	2345.27	74.5000
total path	15561.2	15600.7	83713.6	-0.886393	1.45162	289.333	9.19097
spread	4182.67	4133.33	0.377999e+07	0.296512	-0.301302	1944.22	61.7602
vector range	10977.7	11213.0	0.337993e+07	-0.876502	0.936920	1838.46	58.4006
R-perp			2.127469e+07			4612.45	

vector range distribution function
(histogram channel width 200.00)

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
0	1	1	1	1	4	2	2	1	2	3	2	4	2	8	7	1	8	9	7
14	11	7	16	16	16	27	31	25	29	30	27	37	44	49	46	46	35	52	35
42	59	51	35	36	27	25	16	18	12	5	3	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

penteration distribution function
(histogram channel width 200.00)

0	0	1	0	1	2	0	0	3	1	2	0	2	0	3	0	4	3	2	4
2	2	3	4	3	3	8	8	10	0	5	10	11	10	11	5	12	17	15	9
22	23	25	20	30	28	24	28	38	39	35	37	35	40	23	38	48	38	36	36
40	35	21	24	17	16	8	8	3	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

spread distribution function
(histogram channel width 200.00)

0	2	7	9	15	27	15	21	32	19	30	28	29	26	30	39	34	33	33	37
45	40	44	39	25	26	39	31	26	26	30	25	20	17	21	10	6	8	13	6
5	5	3	1	3	2	2	4	1	1	0	0	2	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

total path distribution function
(histogram channel width 200.00)

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	2	3	10	29	63	142	245	297	174
24	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

be+ ions (901.3 Kev) on u target

ION'S average num. of collisions = 663.
ION'S average num. backscattered = 8.0000e-03

ION'S energy partition

incident (average) =	901.30	
1) - backs. =	1.63	
2) - threshold =	0.02	
3) - elect. (ions) =	862.78	
4) - nuclear (ions)=	36.87	
a) - recial elect. =		5.14
b) - displacement =		29.62
c) - phonon =		2.11
5) - total elect. =		867.91

ALL moving particles : INCIDENT, PRIMARIES, and SECONDARIES will be followed

The Average NUCLEAR Energy loss by an ION = 36.871

39

Subthreshold collisions (Phonon) = 2.114
Net PKAS' energy = 34.757<1><2><4>

(A) Using Lindhard (Robinson) Partition Formula :

Effective Damage Energy = 29.622
Electronic Energy = 5.136

(B) Following the PKAS :

Effective Damage Transfered = 30.323(1)
Electronic Energy Loss = 4.434(1)(2)
Binding Energy Loss = 0.000(1)(2)
Sputtered Energy = 0.000 (2) No. of Sputtered PKAS = 0.00000
Energy lost in replacement = 0.210 (2)
Cut-off Energy = 3.491 (2)
Subthreshold Energy Loss(phonon) = 1.292 (2)
Net Nuclear Energy to Secondaries= 25.331 (2)<3>

sum of [(1)'s] = 34.757<1>
sum of [(2)'s] = 34.757 <2>

The 'Effective Damage Transfered' has the following DISTRIBUION'S PARAMETERS :

total energy in distr. = 30.323

mean	variance	skewness	kurtosis	std dev.	error

357

depth	7512.10	0.963125e+07	-0.491577	-0.625932	3103.43	98.1881
spread	2594.29	0.386771e+07	0.727934	-3.288203e-02	1966.65	62.2220
x	-49.9186	0.492839e+07	-0.138024	0.832251	2220.00	70.2376
u	-2.71521	0.566717e+07	-2.421567e-02	1.09053	2380.58	75.3183
r spread	8123.37	1.067178e+07	-0.616120	-0.544085	3266.77	103.356

average no. of pka's 103.258

(C) FOLLOWING ALL PARTICLES of ALL GENERATIONS :

	including only the SECONDARIES		including SECONDARIES + PKAS	
Electronic Energy Loss =	7.745(3)		12.179(4)	
BINDING Energy Loss =	0.000(3)		0.000(4)	
Phonon Energy Loss =	3.540(3)		4.832(4)	
Sputtered Energy & No. sput. =	0.000(3)	1.000e-03	0.000(4)	1.000e-03
Energy Loss in Replacement =	0.652(3)		0.862(4)	
Cut-off Energy Loss =	13.394(3)		16.885(4)	
sum =	25.331<3>		34.757<4>	

No. of VACANCIES	=	230.312
No. of INTERSTITIALS	=	230.311
No. of (near) V-I	=	192.367
No. of Replacement events	=	64.595
Average No. of PKAS	=	103.
Average No. of cascades	=	85.
Average No. of Atoms in cascades	=	261.
Average No. of ALL moving Atoms	=	364.
maximum cascade storage	=	55

be+ ions (901.3 kev) on u target

** distribution (normalized for 1 particles) **

interval = 200.00

interval no.	coll.	ioniz.	nuclear	displac.	rec-ionz	phonon	dmg/pka	se/pka	se/scnd	V	I	V-I (near)	Rplc
1	0.9	21.6	0.12	0.10	1.68e-02	5.66e-03	0.10	1.49e-02	2.53e-02	0.8	0.8	0.8	0.2
2	0.9	21.6	0.13	0.10	1.80e-02	5.73e-03	0.10	1.65e-02	2.61e-02	0.8	0.8	0.7	0.2
3	1.7	21.4	0.29	0.23	4.93e-02	9.77e-03	0.25	3.98e-02	7.06e-02	1.8	1.8	1.5	0.5
4	1.2	21.4	0.23	0.19	3.58e-02	6.87e-03	0.20	2.91e-02	5.46e-02	1.5	1.5	1.2	0.4
5	1.7	21.2	0.29	0.23	4.86e-02	9.01e-03	0.15	2.60e-02	4.89e-02	1.4	1.4	1.2	0.4
6	1.7	21.3	0.21	0.17	2.96e-02	9.78e-03	0.27	3.01e-02	7.34e-02	1.7	1.7	1.4	0.5
7	1.6	20.8	0.20	0.16	3.13e-02	9.31e-03	0.16	2.28e-02	4.89e-02	1.3	1.4	1.1	0.4
8	1.7	20.4	0.30	0.24	5.08e-02	9.41e-03	0.26	3.30e-02	7.67e-02	1.8	1.8	1.5	0.5
9	2.0	20.3	0.23	0.19	3.40e-02	1.08e-02	0.21	2.54e-02	5.43e-02	1.5	1.5	1.3	0.4
10	2.2	20.2	0.40	0.31	7.06e-02	1.21e-02	0.26	4.14e-02	8.92e-02	2.1	2.0	1.7	0.6
11	2.2	20.0	0.19	0.16	2.58e-02	1.19e-02	0.23	2.41e-02	6.14e-02	1.6	1.6	1.4	0.5
12	1.8	19.8	0.31	0.25	4.71e-02	1.09e-02	0.25	3.60e-02	6.32e-02	1.8	1.8	1.4	0.5
13	1.9	19.6	0.39	0.31	6.60e-02	1.11e-02	0.28	4.56e-02	9.11e-02	2.2	2.2	1.8	0.6
14	2.0	19.3	0.26	0.21	3.74e-02	1.14e-02	0.28	3.30e-02	7.77e-02	2.0	2.0	1.6	0.5
15	2.4	19.0	0.28	0.22	4.23e-02	1.30e-02	0.21	3.19e-02	6.67e-02	1.7	1.8	1.5	0.5
16	2.2	18.9	0.32	0.26	5.22e-02	1.21e-02	0.29	4.29e-02	7.50e-02	2.0	1.9	1.6	0.6
17	2.9	19.0	0.33	0.27	5.25e-02	1.48e-02	0.29	3.56e-02	8.06e-02	2.1	2.1	1.7	0.6
18	3.0	18.5	0.53	0.42	9.80e-02	1.46e-02	0.27	5.53e-02	0.11	2.7	2.7	2.2	0.8
19	3.0	18.2	0.46	0.37	7.72e-02	1.45e-02	0.54	6.79e-02	0.14	3.2	3.2	2.6	0.9
20	3.5	17.9	0.30	0.24	4.08e-02	1.67e-02	0.27	4.02e-02	6.95e-02	2.0	2.1	1.7	0.6
21	3.5	17.7	0.33	0.26	4.75e-02	1.71e-02	0.27	4.13e-02	7.01e-02	2.1	2.1	1.8	0.5
22	3.4	17.3	0.46	0.37	7.41e-02	1.66e-02	0.36	4.89e-02	0.10	2.7	2.6	2.1	0.7
23	3.7	17.3	0.45	0.36	7.02e-02	1.73e-02	0.43	4.83e-02	0.11	2.9	2.9	2.4	0.8
24	3.9	17.2	0.50	0.40	8.15e-02	1.85e-02	0.37	5.45e-02	0.11	2.9	2.9	2.3	0.8
25	4.1	17.0	0.50	0.40	7.70e-02	1.94e-02	0.44	6.07e-02	0.14	3.4	3.4	2.8	1.0
26	4.8	17.1	0.44	0.36	6.52e-02	2.16e-02	0.40	5.10e-02	0.10	2.8	2.8	2.5	0.8
27	6.3	17.0	0.56	0.45	8.41e-02	2.56e-02	0.48	6.73e-02	0.12	3.5	3.4	3.0	1.0
28	7.1	16.6	0.51	0.41	7.48e-02	2.79e-02	0.38	5.61e-02	0.10	3.0	3.1	2.5	0.9
29	6.4	16.2	0.64	0.51	0.10	2.58e-02	0.56	6.82e-02	0.17	4.1	4.1	3.3	1.2
30	4.8	15.9	0.69	0.55	0.11	2.24e-02	0.57	7.89e-02	0.17	4.2	4.2	3.3	1.2
31	5.7	15.7	0.49	0.40	7.03e-02	2.54e-02	0.44	5.81e-02	0.11	3.1	3.1	2.7	0.9
32	6.9	15.5	0.61	0.49	9.42e-02	2.98e-02	0.52	6.60e-02	0.14	3.7	3.7	3.0	1.0
33	8.1	15.4	0.68	0.54	0.10	3.18e-02	0.51	8.40e-02	0.15	4.2	4.1	3.4	1.2
34	7.8	14.9	0.63	0.51	9.15e-02	2.99e-02	0.53	7.15e-02	0.13	3.9	3.9	3.2	1.1
35	9.6	14.2	0.59	0.47	8.12e-02	3.62e-02	0.51	7.84e-02	0.13	3.9	4.0	3.3	1.1
36	9.0	14.0	0.73	0.58	0.10	3.50e-02	0.54	8.06e-02	0.14	4.2	4.2	3.5	1.2
37	9.9	13.7	0.68	0.55	9.79e-02	3.73e-02	0.61	8.12e-02	0.16	4.4	4.4	3.7	1.2
38	11.8	13.2	0.75	0.60	0.10	4.22e-02	0.61	9.14e-02	0.16	4.7	4.7	3.9	1.4
39	11.9	12.9	0.73	0.59	9.94e-02	4.18e-02	0.63	9.05e-02	0.15	4.6	4.6	3.7	1.3
40	12.4	12.8	0.82	0.66	0.11	4.45e-02	0.66	9.82e-02	0.18	5.2	5.2	4.4	1.4
41	13.9	12.4	0.90	0.72	0.12	4.76e-02	0.72	0.10	0.18	5.5	5.5	4.8	1.5
42	16.3	12.1	0.96	0.77	0.13	5.39e-02	0.78	0.11	0.19	5.9	5.8	4.8	1.7
43	17.1	11.7	0.99	0.80	0.13	5.54e-02	0.87	0.12	0.21	6.4	6.5	5.4	1.8
44	17.1	10.9	0.96	0.78	0.13	5.45e-02	0.79	0.11	0.20	6.0	5.9	4.9	1.7
45	18.6	10.2	0.95	0.76	0.12	5.88e-02	0.75	0.11	0.19	6.0	6.0	5.1	1.7

```
 46   20.4   10.2    1.1       0.87       0.14       6.32e-02   0.89       0.13       0.21        6.8   6.7   5.7   1.9
 47   17.6    9.3   0.91       0.73       0.12       5.69e-02   0.74       0.11       0.18        5.8   5.9   4.7   1.7
 48   20.3    9.0    1.0       0.84       0.13       6.23e-02   0.84       0.12       0.20        6.6   6.5   5.4   1.8
 49   22.9    8.2    1.0       0.83       0.13       6.66e-02   0.84       0.12       0.21        6.5   6.5   5.5   1.8
 50   23.7    7.6    1.0       0.81       0.13       6.61e-02   0.81       0.12       0.19        6.3   6.4   5.3   1.8
 51   26.5    7.4   0.98       0.79       0.12       7.20e-02   0.81       0.12       0.18        6.4   6.4   5.3   1.8
 52   23.1    6.7   0.97       0.77       0.12       6.53e-02   0.76       0.11       0.18        6.0   6.0   5.1   1.6
 53   22.5    5.9   0.88       0.71       0.11       6.31e-02   0.73       0.11       0.16        5.7   5.7   4.8   1.6
 54   22.8    5.5   0.92       0.74       0.11       6.19e-02   0.74       0.11       0.17        5.8   5.8   4.9   1.6
 55   21.0    4.6   0.79       0.63       9.76e-02   5.68e-02   0.64       9.88e-02   0.14        5.1   5.1   4.4   1.4
 56   23.3    4.1   0.79       0.63       9.76e-02   6.13e-02   0.64       0.10       0.14        5.0   5.0   4.2   1.4
 57   23.3    3.5   0.79       0.63       9.73e-02   6.01e-02   0.63       0.10       0.14        5.1   5.1   4.3   1.4
 58   23.2    2.9   0.67       0.53       8.07e-02   5.58e-02   0.53       8.60e-02   0.11        4.3   4.2   3.5   1.2
 59   19.2    2.2   0.54       0.43       6.37e-02   4.61e-02   0.42       7.11e-02   8.77e-02    3.5   3.5   3.0   1.0
 60   19.6    1.9   0.49       0.39       5.67e-02   4.55e-02   0.38       6.57e-02   7.38e-02    3.1   3.1   2.7   0.9
 61   16.6    1.4   0.41       0.32       4.72e-02   3.91e-02   0.31       5.35e-02   6.20e-02    2.6   2.6   2.2   0.7
 62   13.2    1.0   0.29       0.23       3.27e-02   3.02e-02   0.23       4.09e-02   4.23e-02    1.9   1.9   1.7   0.5
 63   11.6    0.8   0.25       0.19       2.80e-02   2.54e-02   0.18       3.28e-02   3.36e-02    1.5   1.6   1.3   0.4
 64    8.8    0.5   0.17       0.13       1.87e-02   1.97e-02   0.13       2.25e-02   2.57e-02    1.1   1.1   1.0   0.3
 65    6.1    0.3   0.10       8.16e-02   1.08e-02   1.39e-02   8.03e-02   1.49e-02   1.19e-02    0.7   0.7   0.6   0.2
 66    5.1    0.2   7.29e-02   5.43e-02   6.88e-03   1.16e-02   5.09e-02   9.56e-03   7.18e-03    0.5   0.5   0.4   0.1
 67    4.1    0.1   5.55e-02   4.15e-02   5.36e-03   8.56e-03   4.09e-02   7.47e-03   5.84e-03    0.4   0.4   0.3   0.1
 68    2.1    0.1   2.63e-02   1.96e-02   2.41e-03   4.31e-03   1.90e-02   3.56e-03   2.15e-03    0.2   0.2   0.1   0.0
 69    0.8    0.0   1.33e-02   1.00e-02   1.40e-03   1.86e-03   8.07e-03   1.45e-03   1.78e-03    0.1   0.1   0.1   0.0
 70    0.1    0.0   4.22e-04   2.55e-04   2.55e-05   1.41e-04   1.45e-03   2.01e-04   8.85e-05    0.0   0.0   0.0   0.0
 71    0.2    0.0   2.55e-03   1.88e-03   2.32e-04   4.38e-04   1.68e-03   4.37e-04   1.85e-04    0.0   0.0   0.0   0.0
 72    0.0    0.0   0.00       0.00       0.00       0.00       1.72e-03   1.43e-04   5.15e-04    0.0   0.0   0.0   0.0
 73    0.0    0.0   0.00       0.00       0.00       0.00       0.00       0.00       5.59e-06    0.0   0.0   0.0   0.0
 74    0.0    0.0   0.00       0.00       0.00       0.00       0.00       0.00       2.07e-05    0.0   0.0   0.0   0.0
 75    0.0    0.0   0.00       0.00       0.00       0.00       0.00       0.00       0.00        0.0   0.0   0.0   0.0

sum :  663.   863.   36.9       29.6       5.14       2.11       30.3       4.43       7.74       230.  230.  192.   65.

       backscattered ions energy distribution
       number of histories =  1000   channel width5120.00000 (ev)
   0   1   0   0   0       0   0   1   0   0       0   0   0   0   0       0   0   0   0   1       0   0   0   0   0
   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   1   0   0       0   0   0   0   1
   0   0   0   0   0       0   0   1   0   1       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0
   0   0   0   0   1       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

       sputtered atoms' energy distribution
       number of histories =  1000   channel width  10.00000 (ev)
   0   0   0   0   0       0   1   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0
   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0
   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0
   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0       0   0   0   0   0


       time in seconds =    277.283

        # histr. =    1000   energy(mev) =      0.90  iseed =        84550200738973

 *

                            end  xherad    -    end  xherad
                            end  xherad    -    end  xherad
```

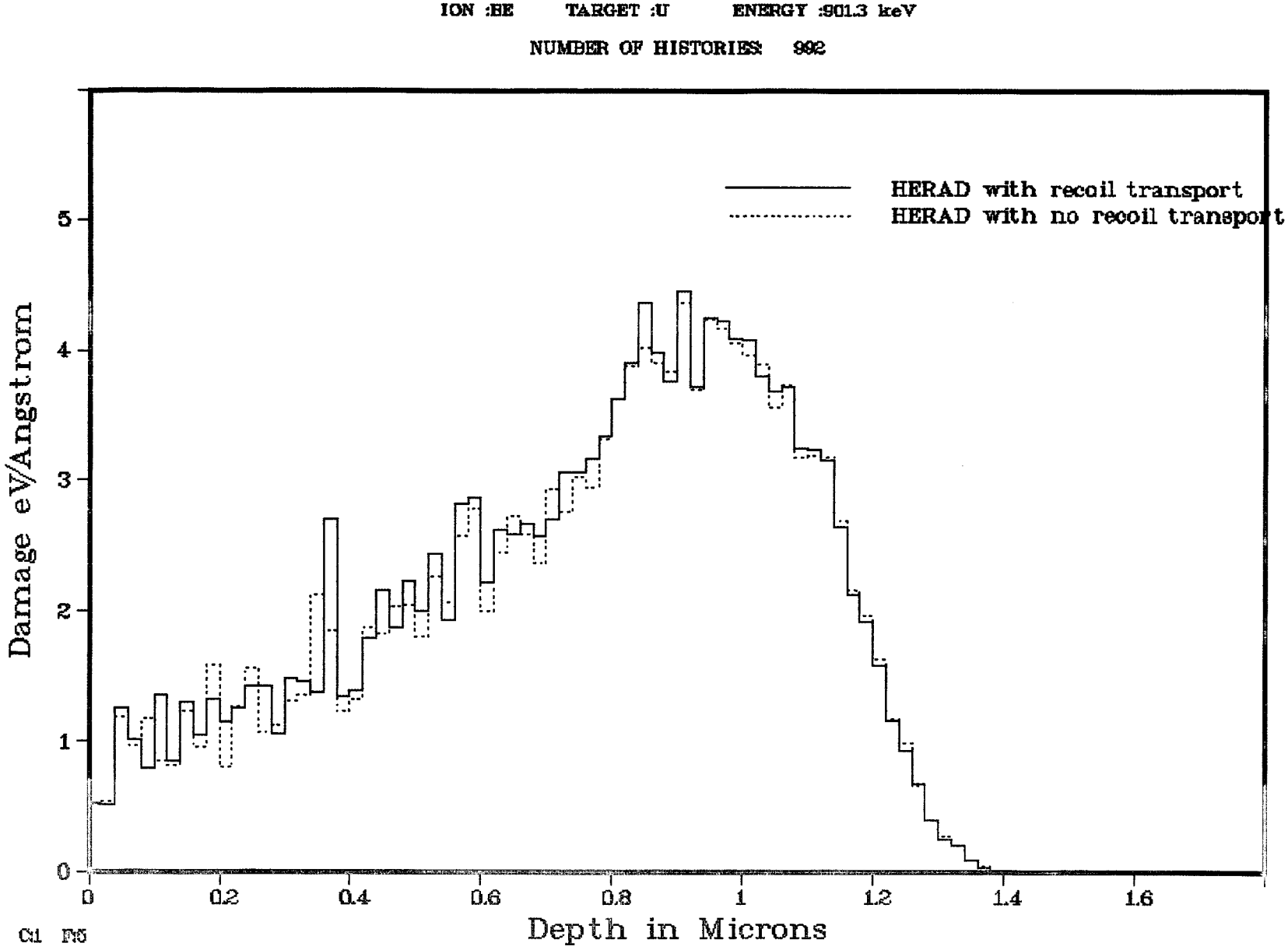
DAMAGE DISTRIBUTIN (HERAD)
ION :BE TARGET :U ENERGY :901.3 keV
NUMBER OF HISTORIES: 992
HERAD with recoil transport
HERAD with no recoil transport
Damage eV/Angstrom
0
1
2
3
4
5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Depth in Microns
C1 F5

Figure 7

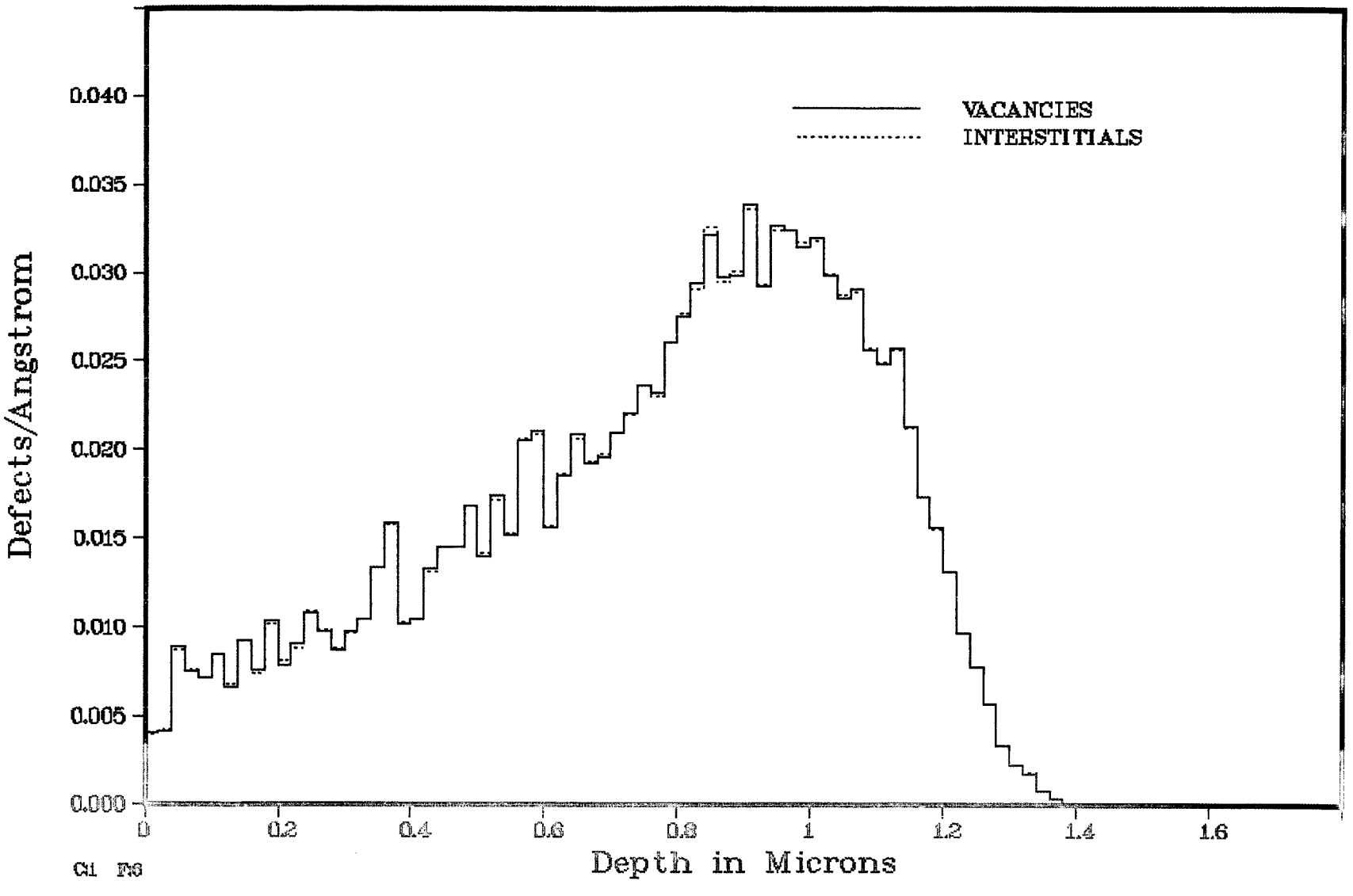
HERAD'S DEFECT DISTRIBUTION
ION :HE TARGET :U ENERGY :901.3 keV
NUMBER OF HISTORIES: 992
VACANCIES
INTERSTITIALS
Defects/Angstrom
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Depth in Microns
C1 F3

Figure 8

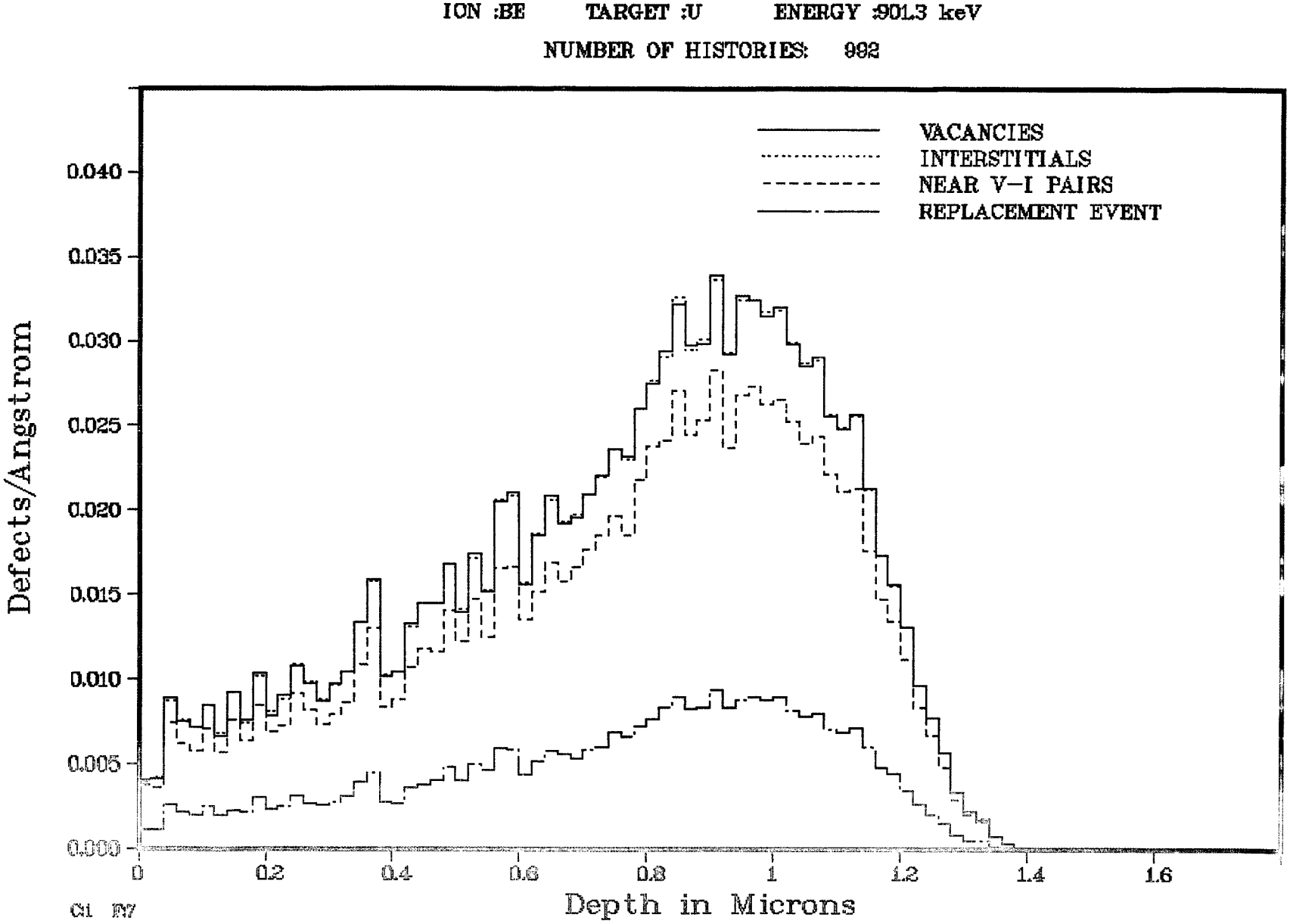
HERAD'S DEFECTS DISTRIBUTION
ION :BE TARGET :U ENERGY :901.3 keV
NUMBER OF HISTORIES: 992
VACANCIES
INTERSTITIALS
NEAR V-I PAIRS
REPLACEMENT EVENT
Defects/Angstrom
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Depth in Microns
C1 E7

Figure 9

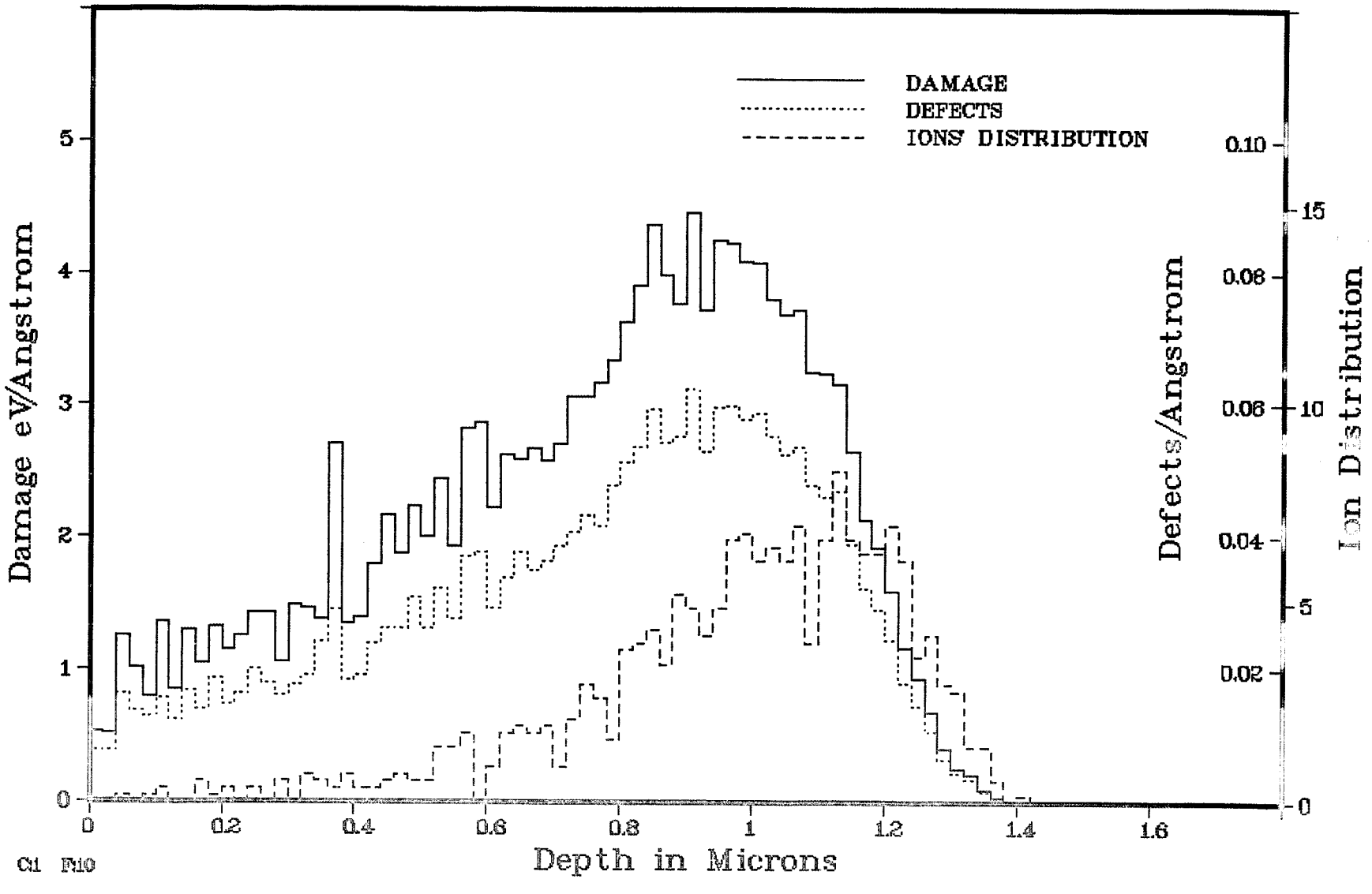
DAMAGE AND IONS' DISTRIBUTIONS
ION :BE TARGET :U ENERGY :901.3 keV
NUMBER OF HISTORIES: 992
DAMAGE
DEFECTS
IONS' DISTRIBUTION
Damage eV/Angstrom
Defects/Angstrom
Ion Distribution
Depth in Microns
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1
2
3
4
5
0.02
0.04
0.06
0.08
0.10
5
10
15
C1 F10

Figure 10

V. Availability of the Code

V.1 Availability of the Code

The HERAD code is available on the NMFECC (National Magnetic Fusion Energy Computer Center, Livermore) computers. The code can be run on the CRAY or the CDC76ØØ computers. The directory c-herad in the FILEM space of user #14225. This directory contains the source file "sherad", the controllee file "xherad" (the executable program), the potentials files mentioned in Section III.3, an input file "ibeu" for the test case described in the next chapter, the output file for the test case "obeuØØ". Also available in this directory the controllee file "xplot" and its input file "iplot".

V.2 Compilation and Loading

The source file sherad contains the cliche "peode" (lines 8-13). This cliche has the parameter "ipltk" which is set to zero. To get a controllee which can direct graphic output to the terminal, set ipltk to a non-zero value. Also in this cliche is the parameter "maxstr" which has a default value of 4ØØ. The parameter is used to set the dimension of the arrays used to store the coordinates and the direction cosines and the initial energy of the displaced secondary atoms in a cascade generated by a primary knockon (PKA) atom. If the number of coils expected exceeds the value of "maxstr", the user should set it to a larger value, otherwise the program will stop if the allowable storage is consumed.

To compile and load the program on the CRAY computers, open the source file "sherad" with the text editor "TRIXGL"[24] and type "run", the program will be "pre-compiled" with "PRECOMP", compiled with the compiler "CFT" and finally loaded with the loader "LDR". On the CDC76ØØ open the source with

"TRIXGL" and move lines 5-6 after line 1 and type "RUN". In this case the "CHATR" routine will compile and load the program.

Before running the controllee ("xherad"), the user should prepare an input file (the default name of this file is "iherad") according to what was described in the last two sections. The user should have also the potential file to be read by the program in his/her disk space. To run the code type

```
xherad i=ifile  /t
```

where "ifile" is the name of the input file and "t" is approximate time estimated for this run.

V.3. Output Files Naming Convention

The second to the sixth characters (maximum of 5 characters) of the name of the input file are used in naming all the output files. These characters are added to the letter "o" or the letter "g" for the name of the output (text) file and the name of the graphic (binary) file respectively. As was mentioned in Section III.1, two characters are added to the names of the output files. The last two characters are a number from Ø to 99, according to the first record in the input file (see Section III.1). Thus if the name of the input file is iabcdefg, the output files will be oabcdeØØ and gabcdeØØ, if the file iabcdefg was read for the first time. If the same input file is used again the names will be oabcdeØ1 and gabcdeØ1, i.e. every time the input file is read the number in the output files is incremented by 1.

Besides these output files, HERAD copies the input file to a log file. This log file will be created if it does not exist in the user's disc space. The purpose of this file, which has the name "<logdamg", is to keep a record for all the cases run by the program.

Acknowledgment

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APPENDIX A. APPLICABILITY OF CLASSICAL MECHANICS

If we wish to apply the classical mechanics to the collision problem, two conditions must be satisfied.[22] The first is that the orbit of the particle must be well-defined in relation to distance, and the second is that the deflection due to the collision must be well defined. The first requires that the DeBroglie wavelength λ of the particle should be less than the minimum dimension associated with the collision. A suitable choice of this distance is the collision diameter b. Thus,

$$\lambda = \frac{\hbar}{M_o v_1} << b \ . \tag{A.1}$$

Defining

$$\chi = \frac{b}{\lambda} \ , \tag{A.2}$$

Eq. (A.2) becomes

$$\chi >> 1 \ . \tag{A.3}$$

The second condition requires that, if Δp is the momentum transfer in the collision, one must have

$$b\Delta p >> \hbar \ . \tag{A.4}$$

Δp is the order of $V(b)/v_1$, and hence we have

$$b \frac{V(b)}{v_1 \hbar} >> 1 \ . \tag{A.5}$$

In terms of the angle of scattering θ, which is of the order $V(b)/M_o v^2$, this condition can be written as $\theta >> \hbar/mva$. Since θ is of the order of unity, and

in case of Coulomb interaction, the first condition, Eq. (A.3), is a necessary and sufficient condition for using classical mechanics, leading to Rutherford scattering.[2]

For the case of minimum screening, i.e. $\xi \ll 1$, $\varepsilon \gg 1$, or minimum distance of separation, and when condition (A.3) is satisfied, classical mechanics can be applied and leads to Rutherford scattering for all angles larger than a minimum angle. This minimum angle corresponds to an impact parameter in the order of the screening length and is given by Bohr[5] to be

$$\theta_{min} \approx \xi = \frac{Z_1 Z_2 e^2}{M_o v_1^2 a} , \tag{A.6}$$

and by Mott and Massey[22] as

$$\theta_{min} = \frac{3.8\ Z_2^{4/3} e^2}{M_o v^2 a_o} . \tag{A.7}$$

If Eq. (A.3) is not fulfilled, i.e. when $\lambda\!\!\!^{-} \geq b$ and still $\xi \ll 1$, i.e. $(b \ll a)$, the Born approximation can be used and there will be a region of scattering angles confined to Rutherford scattering with a minimum angle given by

$$\theta_{min} = \frac{\lambda\!\!\!^{-}}{a} , \qquad \text{(Bohr)}$$

and (A.8)

$$\theta_{min} = 2.1\ Z_2^{1/3} \hbar/(M_o v_1 a_o) . \qquad \text{(Mott and Massey)}$$

In the case of excessive screening, i.e. $b \geq a$, condition (A.3) would not be sufficient for the classical mechanics to be applied, and we require $\lambda \ll a$ rather than $\lambda \ll b$. In this case, it would be impossible to trace angles

smaller than

$$\theta_{min} \approx \frac{\lambda}{a} = \frac{\xi}{\chi} , \tag{A.9}$$

and the scattering will be essentially different from that in the unscreened fields. The scattering then tends towards a spherically symmetrical angular distribution. Thus the condition for classical mechanics to be applied in this case is $\theta_{min} << 1$. From Eq. (A.9), this implies that

$$\chi >> \xi . \tag{A.10}$$

When $\lambda > a$, the quantum mechanics treatment should be used. However, there exists a region where the Born approximation can still be used where $\chi < \lambda/2a$ or

$$\chi << \sqrt{\xi} . \tag{A.11}$$