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ANALYSIS OF TARGETS WITH NONUNIFORM COMPOSITION AS A
FUNCTION OF DEPTH: ELASTIC AND INELASTIC SCATTERING

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ABSTRACT

This paper describes an analytical technique to reduce yield versus energy spectra to impurity concentration versus depth. It applies to both elastic and inelastic reactions and calculates the depth distribution profile directly from the observed data. It uses the experimental spectrum to be analyzed, stopping cross sections and reaction cross sections to obtain the desired depth scales and the depth dependence of the target composition. A computer code, NUCREA, has been developed to perform such analysis. A description of NUCREA, a user's guide, a complete listing and a typical output for the code are contained in the report. An example showing the analysis of experimental data is also presented.

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I. INTRODUCTION

The characterization of solids implanted and diffused with impurity atoms is of concern to a variety of fields. Both nuclear microanalysis and ion backscattering of energetic light ions have proven to be useful tools in the study of thin films and surfaces.^{1,2} Measurements of the depth distribution of the impurity atoms can lead to a greater understanding of the basic physics involved in energy loss, diffusion, oxidation, compound formation and other related phenomena. Light atomic impurities do not readily lend themselves to ion backscattering because the elemental Rutherford cross section at a given energy decreases as the square of the decreasing atomic number. Nuclear reactions therefore have been used to study various phenomena associated with light atom impurity. Oxidation phenomena have been studied^{3,4} using the reactions $^{16}\text{O}(\text{d},\text{p})^{17}\text{O}$ and $^{16}\text{O}(\text{d},\alpha)^{14}\text{N}$ and helium and hydrogen depth distributions were measured⁵ using the reactions $^3\text{He}(\text{d},\text{p})^4\text{He}$ and $\text{D}(^3\text{He},\text{p})^4\text{He}$. Many of the nuclear reactions used in nuclear microanalysis have been summarized and reviewed in previous articles.⁶ Recently the use of ion backscattering to observe D and He had been^{7,8} successfully accomplished. An enhanced elastic scattering cross section was found,⁷ e.g., 260 times the Rutherford scattering cross section for $\text{H} \rightarrow \text{D}$ at 2.8 MeV for $\theta_{\text{lab}} = 170^\circ$. Both D and He depth distributions have been measured in both thin free-standing films and solid substrates.⁷

The present paper describes an analytical technique to reduce yield vs. energy spectra to impurity concentrations vs. depth. It applies to both elastic and inelastic reactions and calculates the depth distribution profile directly from the observed data. Previous analytical techniques for data reduction of nuclear reactions have consisted of calculating an expected spectra for an assumed distribution and comparing that with the observed distribution.⁴ A previous paper by D. K. Brice described a program to analyze backscattering data of targets with nonuniform composition as a function of depth.⁹ It uses the experimental spectrum to be analyzed with an experimental reference spectrum to obtain the desired depth scales and the depth dependence of target composition. The present technique differs from the previous work in that it is applicable to both inelastic and elastic collisions and uses only the experimental spectrum to be analyzed.

A computer code, NUCREA, has been written which implements the extraction of depth distribution information and the construction of energy-to-depth conversion scales for two-atomic component targets from a single experimental spectrum. A description of NUCREA, a complete listing and a user's guide for the code are contained in the present report. In Section II the basic theory is described and the general equation is derived. In Section III a procedure is developed which allows one to use the general equation along with an experimental spectrum to be analyzed to obtain the desired depth scales and depth dependence of the target composition. Section IV through VII present a discussion of the code NUCREA and contain in order a general description, a user's guide, a listing, and typical output from a run.

II. THEORY (Derivation of Yield Equation)

Figure 1 shows the geometry used in a typical large angle reaction experiment, and introduces the notation used in the present report. An incident ion with energy E , mass m_1 and atomic number Z_1 is incident on the surface of a target. The incident velocity vector makes an angle φ with respect to the target surface. At some depth within the target the ion suffers a large angle elastic scattering event or a nuclear reaction event after which the velocity vector of the reactant ion makes an angle θ with respect to the incident ion direction. The energy just before the reaction event is labeled E and just after the event it is E' . For elastic scattering events $E' = KE$ where the kinematic factor K depends on the incident ion mass, m_1 , the scattering mass, m_2 , as well as the scattering angle θ and is given by

$$K = \left\{ \frac{m_1 \cos \theta}{m_1 + m_2} + \left[\left(\frac{m_1 \cos \theta}{m_1 + m_2} \right)^2 + \left(\frac{m_2 - m_1}{m_1 + m_2} \right)^2 \right]^{\frac{1}{2}} \right\}^2 \quad (1)$$

For nuclear reactions where the incident ion nucleus combines with the target atom nucleus to form a compound nucleus which then quickly disintegrates into two reaction products the outgoing energy E' of the observed particle as a function E is given by

$$E' = \frac{1}{2m_4} \left\{ \frac{\cos \theta \pm \{2m_1 E \cos^2 \theta - (1 + \frac{m_3}{m_4})(2m_1 E [1 - \frac{m_3}{m_1}] - 2m_3 Q)\}^{\frac{1}{2}}}{1 - \frac{m_3}{m_1}} \right\}, \quad (2)$$

where m_4 is the observed particle mass, m_3 the other reaction product and Q is the excess energy of the reaction. For light ions incident on thin film targets straggling and multiple scattering effects are usually smaller than the detector resolution. For this reason these effects are not included in the present calculations, although they may be important for targets thicker than $0.3 \mu\text{m}$.

As the observed spectra are collected from a multichannel analyzer, one observes the yield for a particular channel where the collected particle has energy between E' and $E' + \Delta EC$. The one experimental parameter which remains the same throughout the spectra is the energy per channel, ΔEC . As the stopping cross sections for both the incoming and outgoing particles are a function of energy, the thickness layer associated with each energy channel will change accordingly and is defined as a depth channel. Since the energy, E' , of a given reaction product depends on both its instantaneous location within the target as well as the depth at which it was produced the variable E' must be double subscripted. The first subscript on $E'(I, J)$ denotes the depth channel in which the reaction event occurred and the second subscript denotes the last depth channel through which the particle has passed on its path toward the target surface. Emergent particles which have reacted in the thickness $\Delta X(1)$, for example, will have energy between $E'(1, 1)$ and $E'(1, 1) + \Delta EC$ (see Fig. 1).

Fig. 1 - Schematic diagram of geometry for scattering experiment and notation used for data reduction procedure.

The procedure will be to derive the yield formula for the first channel and finally arrive at a general formula for the nth channel. It was found necessary in the actual program to subdivide each channel in cases where the reaction cross section and the stopping cross sections were strong functions of energy because the calculated values for the thickness and composition would vary with methods of calculation. By subdividing each channel it was possible to determine the thickness and composition independent of the calculational method.

The energy relationship for the first channel is given by

$$\Delta EC = E'(2,1) - E'(1,1) \quad (3)$$

$$E'(2,1) + \Delta E'(1,1) = f(E(1) - \Delta E(1)) \approx f(E(1)) - df/dE \Delta E(1) \quad (4)$$

where $E' = f(E)$ as given by Eq. (2), $\Delta E'(1,1)$ is the energy lost by the reaction product in moving from the reaction to the surface (the significant double subscripts are defined above), $E(1)$ is the energy of the particle incident on the first depth channel, and $\Delta E(1)$ is the energy lost by the entering particle as it passes through the first depth channel. (See Fig. 1 for reference.) Solving for $\Delta E'(1,1)$ one obtains

$$\Delta E'(1,1) = -\Delta EC - df/dE \Delta E(1) \quad (5a)$$

and from energy loss considerations

$$\Delta E'(1,1) = S(E'(2,1)) \frac{\Delta X(1)}{\sin(\theta-\varphi)} \quad (5b)$$

where $S(E'(2,1))$ is the stopping cross section of the compound target for the outgoing particle. Eliminating $\Delta E'(1,1)$ from Eqs. (5a) and (5b) one may obtain for $\Delta E(1)$

$$\Delta E(1) = \frac{-\Delta EC - S(E'(2,1)) \Delta X(1)/\sin(\theta-\varphi)}{df/dE} \quad (6a)$$

and from energy loss considerations

$$\Delta E(1) = S(E(1)) \frac{\Delta X(1)}{\sin \varphi} \quad (6b)$$

where $S(E(1))$ is the stopping cross section of the compound target for the incoming particle. The width of depth channel (1), $\Delta X(1)$ can be obtained then from Eqs. (6a) and (6b) by eliminating $\Delta E(1)$ to yield

$$\Delta X(1) = - \frac{\Delta EC}{\frac{S(E(1))}{\sin \varphi} \cdot df/dE + S(E'(2,1))/\sin(\theta-\varphi)} \quad (7)$$

The target is considered to be composed of A atoms and B atoms where the B atoms are the reacting species of the target. The yield, Y, of outgoing particles reacting within depth channel (1) is given by

$$Y(1) = N_B(1) \sigma(E(1)) \Delta L(1) \Omega F \quad (8)$$

where Y is in counts/channel for depth channel (1), $N_B(1)$ the number of reacting target atoms/cm³, σ the reaction cross section, ΔL the thickness in centimeters through which the incident beam passes in traversing depth channel (1), Ω is the geometrical solid angle subtended by the detector and F the fluence of incident ions. It is convenient to have the depth scales in units of A atoms/cm². This conversion is easily made by multiplying ΔX by N_A . One obtains by rearranging Eq. (8)

$$\Delta L(1) = \frac{Y(1)}{R(1) \sigma(E(1)) \Omega F} \quad (9a)$$

Using the geometrical relationship between ΔX and ΔL yields

$$\Delta L(1) = \frac{\Delta X(1)}{\sin \varphi} \quad (9b)$$

where the units of ΔL and ΔX are now A atoms/cm². $R(1)$ is given in (9a) by

$$R(1) = \frac{N_B(1)}{N_A(1)} = \frac{\text{number of B atoms/cm}^3}{\text{number of A atoms/cm}^3} \quad (10)$$

Bragg's Rule is assumed for the relationship between the stopping cross section of the components A and B and the composite target. Thus,

$$S = S_A + R S_B \quad (11)$$

where S_A is the stopping cross section for A atoms and S_B for B atoms and the units for S are eV-cm²/A atoms. Combining Eqs. (7), (8), (9) and (11), one obtains for $R(1)$

$$R(1) = \frac{\frac{Y(1) \sin \varphi}{\sigma(E(1)) \Omega F} \left[\frac{df}{dE} \cdot \frac{1}{\sin \varphi} S_A(E(1)) + \frac{1}{\sin(\theta - \varphi)} S_A(E'(2,1)) \right]}{-\Delta EC - \left[\frac{Y(1) \sin \varphi}{\sigma(E(1)) \Omega F} \right] \left[\frac{df}{dE} \cdot \frac{1}{\sin \varphi} S_B(E(1)) + \frac{1}{\sin(\theta - \varphi)} S_B(E'(2,1)) \right]} \quad (12)$$

Rewriting in a simpler form we obtain

$$B = A[D + F]/(C - A[E + G]) \quad (13)$$

where

$$A = Y(1) \sin \varphi / \sigma(E(1)) \Omega F \quad (14)$$

$$B = R(1) \quad (15)$$

$$C = -\Delta EC \quad (16)$$

$$D = df/dE \cdot S_A(E(1)) / \sin \varphi \quad (17)$$

$$E = df/dE \cdot S_B(E(1)) / \sin \varphi \quad (18)$$

$$F = S_A(E'(2,1)) / \sin(\theta - \varphi) \quad (19)$$

$$G = S_B(E'(2,1)) / \sin(\theta - \varphi) \quad (20)$$

The general formula for the Ith channel is easily derived by iterating the above procedure and may be represented by Eq. (13) with the variables given by

$$A = Y(I) \cdot \sin \varphi / \sigma(E(I)) \cdot \Omega \cdot F \quad (21)$$

$$B = R(I) \quad (22)$$

$$C = -\Delta EC + [\Delta E'(I-1,1) + \dots + \Delta E'(I-1,I-1)] \\ - [\Delta E'(I,1) + \dots + \Delta E'(I,I-1)] \quad (23)$$

$$D = df/dE \cdot S_A(E(I)) \quad (24)$$

$$E = df/dE \cdot S_B(E(I)) \quad (25)$$

$$F = S_A(E'(I+1),I) / \sin(\theta - \varphi) \quad (26)$$

$$G = S_B(E'(I+1),I) / \sin(\theta - \varphi) \quad (27)$$

The second and third terms of Eq. (23) are calculable from stopping powers since the $\Delta X(k)$'s are known for $k \leq I-1$. The general equation (13) is that used for the program NUCREA with the variables given by Eqs. (21) through (27).

III. ANALYSIS OF EXPERIMENTAL DATA

A. General

In this section a procedure will be described which allows the general equation (Eq. (13)) of the previous section to be used in analyzing experimental spectra to obtain information on the depth dependence of target composition. The procedure will be specifically applied to two component targets, although it can easily be applied to the case where the composite target contains more than two types of atoms, but where the various species can be divided into two groups such that within each group the atomic concentrations maintain constant ratio with each other as a function of depth. An example of such a case would be the study of the implantation profile of He in Al_2O_3 where it could be assumed that the atomic ratio of oxygen to aluminum remained constant with depth. For this case the A atoms would be chosen as the host material, Al_2O_3 , and the B atoms as the implanted He atoms.

B. The Iterative Procedure

Experimental spectra are accumulated in discrete energy steps through the use of multichannel analyzers. The analysis of this section explicitly takes this feature of the measurements into account. In addition the experimental spectra generally exhibit statistical scatter approximately 1-3%, and this limits the accuracy of the results through the methods presented here. In principle, however, the analysis is exact.

The discrete energies corresponding to the channels of the multichannel analyzer are denoted by $E'(I,1)$ where I is the channel number. For purposes of the discussion here, I is taken as 1 when E' corresponds to the reactant ions which come from the

target surface. I increases as the depth of the reaction event increases. E' can be increasing or decreasing with I for nuclear reactions, depending upon the geometry of the experiment. For elastic backscattering events E decreases with increasing values of I . It is necessary to be aware that for nuclear reactions certain experimental geometries yield double-valued depth scales.

The iterative procedure begins in channel 1, i.e., the target surface, for those incident ions which have reacted with surface B atoms. The object of the procedure is to determine the ratio of B atoms to A atoms, or $R(I)$, and the thickness of each channel $\Delta X(I)$. After $\Delta X(I)$ has been determined the Eqs. (21) - (27) provide the information necessary to determine $\Delta X(I+1)$. This procedure can be repeated until the spectrum is completely analyzed.

It was found necessary in many cases to subdivide each channel into N_3 integral parts. This is because some of the quantities in Eq. (12) vary strongly from channel to channel. This subdivision is accomplished by using as the yield for the subdivided channel $Y(I)/N_3$ calculating $R(I,J)$ and $\Delta X(I,J)$ where J is the J th division of the I th channel. Upon completion of the calculation for the I th channel an average value for the $R(I)$ is determined from the calculated $R(I,J)$'s. The value for $\Delta X(I)$ is determined by

$$\Delta X(I) = \sum_{J=1}^{N_3} \Delta X(I,J) \quad (28)$$

so that on each successive iteration only these $\Delta X(I)$ values are used. In order to determine a value for N_3 which is sufficiently large to give accurate results it is necessary to do a successive procedure where N_3 is increased, e.g., from 1 to 5 to 10, in order to determine at what value of N_3 the results reach some consistent value. For elastic backscattering events $N_3 = 1$ is usually sufficient, but for nuclear reaction events N_3 is dependent on the energy dependence of the reaction used, the energy dependence of the stopping cross sections of the target, and on the geometry of the experimental setup. For the reaction ${}^3\text{He}(d,p){}^4\text{He}$ a value for $N_3 = 10$ was found to give consistently accurate results.

IV. NUCREA: DESCRIPTIVE

A. General

The computer code NUCREA consists of the main program NUCREA and three subroutines: SPLIFT, SPLINT AND SECALC. Specific input data and formats are described in Section V. A listing of the CDC6600 Fortran version of the program NUCREA and the subroutine SECALC is given in Section VI, and a display of the typical output is contained in Section VII. The subroutines SPLIFT AND SPLINT are described in Ref. 10. The listing is for the general case of inelastic scattering where $Q \neq 0$. The listed version of NUCREA required 106300₈ central memory locations in the computer. This number can be substantially

reduced by limiting the number of channels available for the experimental spectra as described below. The running time for the code depends on the input variables. The time varies roughly as the square of the total number of subchannels to be analyzed. The typical output shown in Section VII required 18 seconds of central memory time for the analysis of 50 channels which were each subdivided into 10 parts. A fast plot routine is included which shows the yield versus channel number and the ratio of B atoms to A atoms versus channel.

Under special conditions the code can be used to analyze targets more complex than two atomic species substrates. These cases are described in more detail in Section III-A. One spectrum is required for use with NUCREA. A total of 100 channels are available for the spectrum. Each of these 100 channels may be subdivided at most into 20 parts. The central memory requirements can be substantially reduced if the total number of channels available for the spectrum is reduced. This is accomplished by replacing the number 100 by the new number of channels in all the dimension statements. The analysis of the spectra begins in the channel corresponding to reaction events occurring at the target surface and proceeds to deeper depths. The analysis terminates at the channel specified by the user in the program.

B. Subroutines

The subroutines SPLIFT and SPLINT are used to fit the input reaction cross section data to a spline and to provide the reaction cross section at any energy within the interval of the data. SPLIFT fits a spline to the N2 data points of the nuclear reaction cross section (EN and SIGMA) and returns the first and second derivatives YP, YPP. The resulting spline defined by the arrays X, Y, and YPP may then be interpolated using SPLINT. SPLINT interpolates and twice differentiates the cubic spline defined by X, Y and YP.

The subroutine SECALC calculates the stopping cross sections required in the analysis. The routine uses the 3-parameter Brice formula¹¹ to obtain the stopping cross section, SE and therefore requires an input of the three parameters Z, A and EN for each of the two components of the target and the incident and exit ions. These parameters are stored in the locations ZIA, AIA, ENIA, ZIB, AIB, ENIB, where I = 1 refers to the incoming incident ion; I = 2 refers to the exiting ion; A represents the host target atoms, and B represents the reacting impurity atoms. Since the three parameters have not as yet been determined for every ion-target combination, the user may wish to replace SECALC with an alternate calculation of the stopping cross section. The alternate routine must return a value for SE in $\text{keV-cm}^2/\text{atom}$ for an input energy E in keV. The other arguments in SECALC identify the ion-target atom combination and may be altered in an alternate version of SECALC. The arguments are incident ion atomic number, Z1; target atom atomic number, ZA or ZB; incident ion mass in amu, P1; incident energy in keV, E; stopping cross section in $\text{keV-cm}^2/\text{atom}$, SE; and the three parameters of the stopping cross section formula, Z, A, EN.

C. Output

Typical data from a run of NUCREA is shown in Section VII. All input information is output in a format which explains the nature of the calculation. The input reaction cross section data in the center-of-mass system is given in units of 10^{-27} cm^2 and the output data for the nuclear reaction cross section in the lab system is given in cm^2 . After printing the initial input variables the calculated values of N_B/N_A , $R(I,J)$, for each subdivided channel are printed. The number of columns is equal to the number of subdivisions of the channel. This allows one to estimate the effect on N_B/N_A of the energy dependence of the nuclear reaction cross section and the stopping cross sections. The final output data is shown in an 8-column format for each channel, the first column contains the channel number, the second column is the yield for that channel, the third column the ion energy incident on that channel, the 4th column the energy of the observed particle immediately after the reaction, the 5th column the thickness of that channel in A atoms/ cm^2 , the 6th column the total thickness to that channel in A atoms/ cm^2 , the 7th column the thickness the incident particle covers in getting to that channel, and the final column the ratio of the number of B atoms to the number of A atoms in that channel.

V. NUCREA: USER'S GUIDE

A. Input

The input to NUCREA comprises 10 data cards, and two decks of cards containing respectively the spectrum to be analyzed and the reaction cross section. These cards are described in detail below:

Card 1 FORMAT (8A10)

DATA: (TT(I), I = 1 , 8)

This card contains alphanumeric data which will be printed as a title to the output. Any information the user wishes may be entered on this card.

Card 2 FORMAT (8F5.3)

DATA: Z1, Z2, Z3, Z4, M1, M2, M3, M4

Z1 is the incident ion atomic number

Z2 is the reacting target atom atomic number.

Z3 is the unobserved reactant atomic number.

Z4 is the observed reactant atomic number.

M1 is the incident ion mass in atomic mass units.

M2 is the reacting target mass.

M3 is the unobserved reactant mass.

M4 is the observed reactant mass.

Card 3 FORMAT (2F5.3)

DATA: ZA, ZB

ZA is the atomic number of the A atoms.

ZB is the atomic number of the B atoms.

Card 4 FORMAT (2F10.3)

DATA: THETA, PHI

THETA is the angle the observed emergent particle makes with respect to the incident ion direction.

PHI is the angle between the incident ion beam and the surface of the substrate.

Card 5 FORMAT (3F10.3, E10.3)

DATA: EP(1,1), DEC, Q, CON

EP(1,1) is the mean energy of the observed reacted particles for the surface channel in keV

DEC is the energy/channel in keV

Q is the excess energy in the nuclear reaction in keV.

CON, a constant for a particular spectra, is given as $1/\sigma F$ and has units of $[\text{ster-atoms}]^{-1}$

Card 6 FORMAT (3I5)

DATA: N1, N2, N3

N1 is the number of channels to be analyzed.

N2 is the number of data points to be entered for the nuclear reaction cross section.

N3 is the number of subdivisions for each channel.

Card 7 FORMAT (3F10.4)

DATA: Z1A, A1A, EN1A

The variables Z1A, A1A and EN1A are respectively the parameter Z, A, and EN for use with the Brice stopping power formula where 1 refers to the incident ion and A refers to atoms of type A. If the subroutine SECALC is altered so that the stopping powers are obtained through some other method this card can be omitted.

Card 8 FORMAT (3F10.4)

DATA: Z1B, A1B, EN1B

The variables for this card are the same as for card 7 but for the incident ion on B type atoms.

Card 9 FORMAT (3F10.4)

DATA: Z4A, A4A, EN4A

The variables for this card are the same as for card 7 but for the observed reactant particle on A type atoms.

Card 10 FORMAT (3F10.4)

DATA: Z4B, A4B, and EN4B

The variables for this card are the same as for Card 7 except for the emerging reactant particle on B type atoms.

CARD DECK 1

FORMAT (16F5.0)

DATA: Y(I), Y(I+1), . . . Y(I+15)

This deck contains the spectrum to be analyzed. The variable I through I + 15 are the experimental channel numbers. The yields (Y) should be in order with Y(1) corresponding to the yield for reactions in the surface region of the substrate.

CARD DECK 2

Card 1 FORMAT (8A10)

DATA: (TF(I), I = 1,8)

This card contains alphanumeric data which will be printed as a title to the nuclear reaction cross section output.

Card 2 to N2 + 1

FORMAT (2F10.0)

DATA: EN(J), SIGMA (J), J = 1, N2

This deck contains the energy and its associated reaction cross section in the center-of-mass system, the units are keV and 10^{-27}cm^2 respectively; the data should be entered in ascending energy order.

The program converts the cross section in the center-of-mass system to the cross section in the lab system.

VI. NUCREA: LISTING

This section contains a listing of the CDC 6600 version of NUCREA. This version requires 106300₈ central memory locations. Running time for the analysis of 60 channels subdivided into 10 parts for target-containing A and B atoms is approximately 20 seconds. Running time varies roughly as the square of the total number of subdivided channels analyzed. To use the program for elastic scattering, i.e., $Q = 0$, it is necessary only to replace lines 72 through 76 with the statements $H(Z) = EPP/K$ and $DEPDE(Z) = K$ where K is determined by Eq. (1).

PROGRAM NUCREA(INPUT,OUTPUT,TAPE10)	NUCREA	2
*****	NUCREA	3
*****	NUCREA	4
*****	NUCREA	5
* ISSUED BY SANDIA LABORATORIES.	* NUCREA	6
*****	NUCREA	7
*****	NUCREA	8
*****	NUCREA	9
* A PRIME CONTRACTOR TO THE	* NUCREA	10
*****	NUCREA	11
*****	NUCREA	12
*****	NUCREA	13
* THIS REPORT WAS PREPARED AS AN ACCOUNT OF WORK SPONSORED BY THE	* NUCREA	14
*****	NUCREA	15
* UNITED STATES GOVERNMENT. NEITHER THE UNITED STATES NOR THE	* NUCREA	16
*****	NUCREA	17
* ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION, NOR ANY OF THEIR	* NUCREA	18
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* OR USEFULNESS OF ANY INFORMATION, APPARATUS, PRODUCT OR PROCESS	* NUCREA	26
*****	NUCREA	27
* DISCLOSED, OR REPRESENTS THAT ITS USE WOULD NOT INFRINGE	* NUCREA	28
*****	NUCREA	29
* PRIVATELY OWNED RIGHTS.	* NUCREA	30
*****	NUCREA	31
*****	NUCREA	32
*****	NUCREA	33
* THE BASIC REFERENCE DOCUMENT FOR THIS CODE IS SLA 75-0331.	* NUCREA	34
*****	NUCREA	35
*****	NUCREA	36
*****	NUCREA	37
* THIS CODE IS FOR UNITED STATES DISTRIBUTION ONLY. NO FOREIGN	* NUCREA	38
*****	NUCREA	39
* DISSEMINATION IS PERMITTED WITHOUT SPECIFIC WRITTEN PERMISSION	* NUCREA	40
*****	NUCREA	41
* FROM SANDIA LABORATORIES, ALBUQUERQUE, N. M. 87115	* NUCREA	42
*****	NUCREA	43
*****	NUCREA	44
*****	NUCREA	45
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DEE=ENERGY/CHANNEL	NUCREA	52
N1=NUMBER OF DATA POINTS	NUCREA	53
N2=NUMBER OF NUCLEAR CROSS SECTION DATA POINTS	NUCREA	54
N3=NUMBER OF POINTS TO BE CALCULATED/CHANNEL FOR SUBDIVIDED SCALE	NUCREA	55
A AND H DENOTE SUBSTRATE COMPONENTS FOR SUBROUTINE SELAC	NUCREA	56
THETA=SCATTERING ANGLE	NUCREA	57
PHI=ANGLE OF ATTACK, SUBSTRATE SURFACE TO ION BEAM	NUCREA	58
TI=SPECTRA TITLE	NUCREA	59
TS=NUCLEAR CROSS SECTION TITLE	NUCREA	60
DIMENSION OF (EN,SIGMA,YP,YPP) TO BE NO. OF DATA PTS., W DIM. 3*	NUCREA	61
REAL L	NUCREA	62
REAL M1,M2,M3,M4	NUCREA	63
DIMENSION EP(100,20),E(100,20),DE(100,20),TP(100,20),DEE(100),	NUCREA	64
*DX(100,20),X(100,20),L(100,20),R(100,20),Y(100),RR(100),YZ(100),	NUCREA	65
*EN(100),SIGMA(100),YP(100),YPP(100),W(300)	NUCREA	66
DIMENSION TI(8),TS(8)	NUCREA	67
DIMENSION ATITLE(6),OTITL1(6),OTITL2(6),CH(100)	NUCREA	68
DATA (ATITLE(I),I=1,6)/1H,1H,7HCHANNEL,1H,1H,1H /	NUCREA	69
DATA (OTITL1(I),I=1,6)/1H,1H,5HOLEIY,1H,1H,1H /	NUCREA	70
DATA (OTITL2(I),I=1,6)/1H,1H,5HAN/RN,1H,1H,1H /	NUCREA	71
F(7)=((SORT(2.0*M4*Z)*COSI+SORT((2.0*M4*Z*(COSI**2)+(1.0-M3/M1)	NUCREA	72
2.0*M3*Q-(2.0*M4*Z)*(1.0*M3/M4))))/(1.0-M3/M1)2/(2.0*M1)	NUCREA	73

DEPDF(Z)=(SQRT(M1*EPP)/SQRT(M4*Z))*((SQRT(M4*EPP)*COST	NUCREA	74
*-SQRT(M1*Z)*(1.0-M3/M1))/(SQRT(M4*EPP)*(1.0+M3/M4)-SQRT(M1*Z)	NUCREA	75
**COST))	NUCREA	76
CALL HOCOPY(10)	NUCREA	77
READ 215,(TT(I),I=1,8)	NUCREA	78
PRINT 214	NUCREA	79
PRINT 215,(TT(I),I=1,8)	NUCREA	80
PRINT 350	NUCREA	81
READ 200,Z1,Z2,Z3,Z4,M1,M2,M3,M4	NUCREA	82
READ 200,ZA,ZB	NUCREA	83
READ 201,THEIA,PHI	NUCREA	84
READ 202,EP(1,1),DEC,U,CON	NUCREA	85
READ 203,N1,M2,N3	NUCREA	86
READ 204,Z1A,A1A,EN1A	NUCREA	87
READ 204,Z1B,A1B,EN1B	NUCREA	88
READ 204,Z4A,A4A,EN4A	NUCREA	89
READ 204,Z4B,A4B,EN4B	NUCREA	90
PRINT 362	NUCREA	91
PRINT 363,PHI,THEIA	NUCREA	92
PRINT 351	NUCREA	93
PRINT 360	NUCREA	94
PRINT 361,Z1,Z2,Z3,Z4,M1,M2,M3,M4	NUCREA	95
PRINT 351	NUCREA	96
PRINT 372	NUCREA	97
PRINT 351,ZA,ZB	NUCREA	98
PRINT 351	NUCREA	99
PRINT 364	NUCREA	100
PRINT 365,DEC,U,CON	NUCREA	101
PRINT 351	NUCREA	102
PRINT 350	NUCREA	103
PRINT 365	NUCREA	104
PRINT 367,Z1A,A1A,EN1A	NUCREA	105
PRINT 367,Z1B,A1B,EN1B	NUCREA	106
PRINT 367,Z4A,A4A,EN4A	NUCREA	107
PRINT 367,Z4B,A4B,EN4B	NUCREA	108
PRINT 1	NUCREA	109
102 READ 206,(Y(J),J=1,N1)	NUCREA	110
PRINT 350	NUCREA	111
PRINT 371	NUCREA	112
PRINT 305,(J,Y(J),J=1,N1)	NUCREA	113
PRINT 1	NUCREA	114
SINT=SIN(THETA)	NUCREA	115
SIMP=SIN(PHI)	NUCREA	116
SINTP=SIN(THETA-PHI)	NUCREA	117
COST=COS(THETA)	NUCREA	118
AN3=N3	NUCREA	119
AN4=N4	NUCREA	120
PRINT 350	NUCREA	121
READ 215,(IS(I),I=1,8)	NUCREA	122
PRINT 215,(IS(I),I=1,8)	NUCREA	123
EN=LAB ENERGY OF INCIDENT PARTICLE,SIGMA=CENTER OF MASS SIGMA	NUCREA	124
PRINT 351	NUCREA	125
READ 205,(EN(J),SIGMA(J),J=1,N2)	NUCREA	126
PRINT 355	NUCREA	127
PRINT 369,(EN(I),SIGMA(I),I=1,N2)	NUCREA	128
DO 101 I=1,N2	NUCREA	129
AP=M1*M4*EN(I)/((M1*M2)*(M3*M4)*(EN(I)+Q))	NUCREA	130
CP=AP*M3/M4	NUCREA	131
CP=M2*M3*(1+(M1*Q/(M2*(EN(I)+Q)))/((M1*M2)*(M3*M4))	NUCREA	132
CP=CP*M4/M3	NUCREA	133
SIGMA(I)=SIGMA(I)*(AP*(COST+SQRT(CP/AP-(SINT)**2))**2)/(SQRT(AP*CP	NUCREA	134
)*SQRT(CP/AP-(SINT)**2))	NUCREA	135
SIGMA(I)=SIGMA(I)*(1.0E-27)	NUCREA	136
101 CONTINUE	NUCREA	137
PRINT 350	NUCREA	138
PRINT 370	NUCREA	139
PRINT 369,(EN(I),SIGMA(I),I=1,N2)	NUCREA	140
PRINT 1	NUCREA	141
CALL SPLITF(EN,SIGMA,YP,YPP,N2,W,IERR,0,0,0,0,0)	NUCREA	142
EPP=EP(1,1)	NUCREA	143
E(1,1)=E(EPP)	NUCREA	144
EP(1,2)=P(1,1)+DEC/AN3	NUCREA	145

DF=DEPDE(E(1,1))	NUCREA	146
EPP=EP(1,2)	NUCREA	147
CALL SPLINT(FN,SIGMA,YPP,N2,E(1,1),SIG,YPI,YMPI,1,KERR)	NUCREA	148
CALL SECALC(Z1,ZA,M1,E(1,1),SE1,Z1A,A1A,EN1A)	NUCREA	149
CALL SECALC(Z1,ZB,M1,E(1,1),SE2,Z1B,A1B,EN1B)	NUCREA	150
CALL SECALC(Z4,ZA,M4,EPP,SE3,Z4A,A4A,EN4A)	NUCREA	151
CALL SECALC(Z4,ZB,M4,EPP,SE4,Z4B,A4B,EN4B)	NUCREA	152
A=CON*SINP*Y(1)/(SIG*AN3)	NUCREA	153
C=-DEC/AN3	NUCREA	154
D=DF*SE1/SINP	NUCREA	155
EE=DF*SE2/SINP	NUCREA	156
F=SE3/SINP	NUCREA	157
G=SE4/SINP	NUCREA	158
H=(A*D+A*F)/(C-A*EE-A*G)	NUCREA	159
X(1,1)=H	NUCREA	160
DX(1,1)=C/(D+H*EE+F+H*G)	NUCREA	161
X(1,1)=DX(1,1)	NUCREA	162
L(1,1)=X(1,1)/SINP	NUCREA	163
DE(1,1)=DX(1,1)*(SE3+H*SE4)/SINP	NUCREA	164
TP(1,1)=DX(1,1)*(SE3+H*SE4)/SINP	NUCREA	165
FPP=EP(1,2)+TP(1,1)	NUCREA	166
TP(03,09,1) GO TO 115	NUCREA	167
DO 103 J=2,N3	NUCREA	168
E(1,J)=H(FPP)	NUCREA	169
EP(1,J+1)=EP(1,J)+DEC/AN3	NUCREA	170
FPP=EP(1,J+1)	NUCREA	171
M=J-1	NUCREA	172
DO 104 K=1,M	NUCREA	173
CALL SECALC(Z4,ZA,M4,EPP,SE5,Z4A,A4A,EN4A)	NUCREA	174
CALL SECALC(Z4,ZB,M4,EPP,SE6,Z4B,A4B,EN4B)	NUCREA	175
DUM=DX(1,K)*(SE5+X(1,K)*SE6)/SINP	NUCREA	176
104 FPP=FPP+DUM	NUCREA	177
TP(1,J)=FPP-EP(1,J+1)	NUCREA	178
CALL SPLINT(FN,SIGMA,YPP,N2,E(1,J),SIG,YPI,YMPI,1,KERR)	NUCREA	179
CALL SECALC(Z1,ZA,M1,E(1,J),SE1,Z1A,A1A,EN1A)	NUCREA	180
CALL SECALC(Z1,ZB,M1,E(1,J),SE2,Z1B,A1B,EN1B)	NUCREA	181
CALL SECALC(Z4,ZA,M4,EPP,SE3,Z4A,A4A,EN4A)	NUCREA	182
CALL SECALC(Z4,ZB,M4,EPP,SE4,Z4B,A4B,EN4B)	NUCREA	183
DF=DEPDE(E(1,J))	NUCREA	184
A=CON*SINP*Y(1)/(SIG*AN3)	NUCREA	185
C=-(DEC/AN3)+TP(1,J-1)-TP(1,J)	NUCREA	186
D=DF*SE1/SINP	NUCREA	187
EE=DF*SE2/SINP	NUCREA	188
F=SE3/SINP	NUCREA	189
G=SE4/SINP	NUCREA	190
H=(A*D+A*F)/(C-A*EE-A*G)	NUCREA	191
X(1,J)=H	NUCREA	192
DX(1,J)=C/(D+H*EE+F+H*G)	NUCREA	193
DE(1,J)=DX(1,J)*(SE1+X(1,J)*SE2)/SINP	NUCREA	194
X(1,J)=X(1,J-1)+DX(1,J)	NUCREA	195
L(1,J)=X(1,J)/SINP	NUCREA	196
TP(1,J)=TP(1,J)+(DX(1,J)*(SE3+X(1,J)*SE4)/SINP)	NUCREA	197
103 FPP=EP(1,J+1)+TP(1,J)	NUCREA	198
115 CONTINUE	NUCREA	199
YZ(1)=Y(1)/AN3	NUCREA	200
IF (N3,09,1) GO TO 116	NUCREA	201
TP(1,1)=TP(1,N3)	NUCREA	202
DX(1,1)=X(1,N3)	NUCREA	203
X(1,1)=X(1,N3)	NUCREA	204
L(1,1)=X(1,1)/SINP	NUCREA	205
116 EP(2,1)=EP(1,N3+1)	NUCREA	206
FPP=EP(2,1)	NUCREA	207
DUM=0.0	NUCREA	208
DO 105 K=1,N3	NUCREA	209
105 DUM=DUM+X(1,K)	NUCREA	210
RR(1)=DUM/AN3	NUCREA	211
CALL SECALC(Z4,ZA,M4,EPP,SE5,Z4A,A4A,EN4A)	NUCREA	212
CALL SECALC(Z4,ZB,M4,EPP,SE6,Z4B,A4B,EN4B)	NUCREA	213
TP(1,1)=DX(1,1)*(SE5+RR(1)*SE6)/SINP	NUCREA	214
FPP=EP(2,1)+TP(1,1)	NUCREA	215
DO 113 I=2,N1	NUCREA	216

DO 106 J=1,N3	NUCREA	217
E(I,J)=H(EPP)	NUCREA	218
EP(I,J+1)=EP(I,J)+DEC/AN3	NUCREA	219
EPP=EP(I,J+1)	NUCREA	220
M=J-1	NUCREA	221
DO 117 K=1,M	NUCREA	222
CALL SECALC(Z4,ZA,M4,EPP,SE5,Z4A,A4A,EN4A)	NUCREA	223
CALL SECALC(Z4,ZB,M4,EPP,SE6,Z4B,A4B,EN4B)	NUCREA	224
DUM=DX(K,1)*(SE5+RR(K)*SE6)/SINTP	NUCREA	225
117 EPP=EPP+DUM	NUCREA	226
IF (J.EQ.1) GO TO 108	NUCREA	227
M=J-1	NUCREA	228
DO 107 K=1,M	NUCREA	229
CALL SECALC(Z4,ZA,M4,EPP,SE5,Z4A,A4A,EN4A)	NUCREA	230
CALL SECALC(Z4,ZB,M4,EPP,SE6,Z4B,A4B,EN4B)	NUCREA	231
DUM=DX(I,K)*(SE5+R(I,K)*SE6)/SINTP	NUCREA	232
107 EPP=EPP+DUM	NUCREA	233
TP(I,J)=EPP-EP(I,J+1)	NUCREA	234
C=-(DEC/AN3)+TP(I,J-1)-TP(I,J)	NUCREA	235
GO TO 109	NUCREA	236
108 TP(I,1)=EPP-EP(I,2)	NUCREA	237
C=-(DEC/AN3)+TP(I-1,1)-TP(I,1)	NUCREA	238
109 CALL SPLINT(EW,SIGMA,YPP,N2,E(I,J),SIG,YPI,YPI,1,KERR)	NUCREA	239
CALL SECALC(Z1,Z4,M1,E(I,J),SE1,Z1A,A1A,EN1A)	NUCREA	240
CALL SECALC(Z1,Z6,M1,E(I,J),SE2,Z1B,A1B,EN1B)	NUCREA	241
CALL SECALC(Z4,ZA,M4,EPP,SE3,Z4A,A4A,EN4A)	NUCREA	242
CALL SECALC(Z4,ZB,M4,EPP,SE4,Z4B,A4B,EN4B)	NUCREA	243
DE=DEPUE(E(I,J))	NUCREA	244
A=CON*SINP*Y(I)/(SIG*AN3)	NUCREA	245
D=DE*SE1/SINP	NUCREA	246
EE=DE*SE2/SINP	NUCREA	247
F=SE3/SINP	NUCREA	248
G=SE4/SINP	NUCREA	249
H=(A*D+A*F)/(C-A*EE-A*G)	NUCREA	250
R(I,J)=H	NUCREA	251
DX(I,J)=C/(D+B*EE+F+R*G)	NUCREA	252
IF (J.EQ.1) GO TO 118	NUCREA	253
X(I,J)=X(I,J-1)+DX(I,J)	NUCREA	254
GO TO 111	NUCREA	255
118 X(I,J)=X(I-1,N3)+DX(I,J)	NUCREA	256
111 DE(I,J)=DX(I,J)*(SE1+R(I,J)*SE2)/SINP	NUCREA	257
L(I,J)=X(I,J)/SINP	NUCREA	258
TP(I,J)=TP(I,J)+(DX(I,J)*(SE3+R(I,J)*SE4)/SINTP)	NUCREA	259
106 EPP=EP(I,J+1)+TP(I,J)	NUCREA	260
YZ(I)=Y(I)/AN3	NUCREA	261
DX(I,1)=X(I,N3)-X(I-1,N3)	NUCREA	262
X(I,1)=DX(I,1)+X(I-1,1)	NUCREA	263
L(I,1)=X(I,1)/SINP	NUCREA	264
EP(I+1,1)=EP(I,N3+1)	NUCREA	265
EPP=EP(I+1)+TP(I,1)	NUCREA	266
DUM=0.0	NUCREA	267
DO 112 J=1,N3	NUCREA	268
112 DUM=DUM+R(I,J)	NUCREA	269
RR(I)=DUM/AN3	NUCREA	270
EPP=EP(I+1,1)	NUCREA	271
DO 120 K=1,1	NUCREA	272
CALL SECALC(Z4,ZA,M4,EPP,SE5,Z4A,A4A,EN4A)	NUCREA	273
CALL SECALC(Z4,ZB,M4,EPP,SE6,Z4B,A4B,EN4B)	NUCREA	274
DUM=DX(K,1)*(SE5+RR(K)*SE6)/SINTP	NUCREA	275
120 EPP=EPP+DUM	NUCREA	276
TP(I,1)=EPP-EP(I+1,1)	NUCREA	277
113 CONTINUE	NUCREA	278
PRINT 351	NUCREA	279
PRINT 307	NUCREA	280
PRINT 308,(I,(R(I,J),J=1,N3),I=1,N1)	NUCREA	281
PRINT 1	NUCREA	282
PRINT 309	NUCREA	283
PRINT 310	NUCREA	284
J=1	NUCREA	285
PRINT 311,(I,Y(I),E(I,1),EP(I,1),DX(I,1),X(I,1),L(I,1),RR(I),	NUCREA	286

*I=1,N1)	NUCREA	287
DO 131 K=1,N1	NUCREA	288
AK=K	NUCREA	289
131 CH(K)=AK	NUCREA	290
XL=0.0	NUCREA	291
XN1=N1	NUCREA	292
XU=XN1*5.0	NUCREA	293
CALL AICRT3(0.0,CH,Y,N1,1.1,2.1H*,TT,ATITLE,OTITL1,1.1,256.,256.,	NUCREA	294
*2,XL,XU,1,YL,YU)	NUCREA	295
CALL AICRT3(0.0,CH,PR,N1,1.1,2.1H*,TT,ATITLE,OTITL2,1.1,256.,256.,	NUCREA	296
*2,XL,XU,1,YL,YU)	NUCREA	297
CALL EXTFLM(0)	NUCREA	298
INPUT FORMATS (200)	NUCREA	299
1 FORMAT (1H1)	NUCREA	300
200 FORMAT (8F5.3)	NUCREA	301
201 FORMAT (2F10.3)	NUCREA	302
202 FORMAT (3F10.3,E10.3)	NUCREA	303
203 FORMAT (3I5)	NUCREA	304
204 FORMAT (3F10.4)	NUCREA	305
205 FORMAT (2F10.0)	NUCREA	306
206 FORMAT (16F5.0)	NUCREA	307
214 FORMAT (1H1)	NUCREA	308
215 FORMAT (8A10)	NUCREA	309
OUTPUT FORMATS (300)	NUCREA	310
302 FORMAT (5X,1HI,6X,SHYIELD,8X,1HE,11X,2HEP,12X,2HDX,14X,	NUCREA	311
*1HX,14X,1HL,13X,SHNB/NA)	NUCREA	312
303 FORMAT (2X,7HCHANNEL,2X,11HSUB-CHANNEL,5X,5HCOUNT,7X,3HKEV,9X,	NUCREA	313
*3HKEV,4X,11HA-ATOMS/CM2,4X,11HA-ATOMS/CM2,4X,11HA-ATOMS/CM2,77)	NUCREA	314
304 FORMAT (1H,16,2X,16,8X,F8.2,3X,E10.3,3X,E10.3,7X,E10.3,5X,E10.3,	NUCREA	315
*5X,E10.3,5X,E10.3)	NUCREA	316
305 FORMAT (5X,12,4X,E10.3)	NUCREA	317
306 FORMAT (5X,11E10.3)	NUCREA	318
307 FORMAT (4X,1HI,7X,9HR(I,1-N3))	NUCREA	319
308 FORMAT (8X,12,6X,10F7.3)	NUCREA	320
309 FORMAT (5X,1HI, 4X,SHYIELD,8X,1HE,11X,2HEP,12X,2HDX,14X,1HX,14X,	NUCREA	321
*1HL,13X,SHNB/NA)	NUCREA	322
310 FORMAT (2X,7HCHANNEL,5X,5HCOUNT,7X,3HKEV,9X,3HKEV,8X,	NUCREA	323
*11HA-ATOMS/CM2,4X,11HA-ATOMS/CM2,4X,11HA-ATOMS/CM2,77)	NUCREA	324
311 FORMAT (1H,16,2X,F8.2,3X,E10.3,3X,E10.3,7X,E10.3,5X,E10.3,	NUCREA	325
*5X,E10.3,5X,E10.3)	NUCREA	326
350 FORMAT (77777)	NUCREA	327
351 FORMAT (777)	NUCREA	328
360 FORMAT (5X,2HZ1,8X,2HZ2,8X,2HZ3,8X,2HZ4,8X,2HM1,8X,2HM2,8X,2HM3,8X,	NUCREA	329
*2HM4)	NUCREA	330
361 FORMAT (8(2X,F8.4))	NUCREA	331
362 FORMAT (5X,1SHANGLE OF ATTACK,10X,16HSCATTERING ANGLE)	NUCREA	332
363 FORMAT (5X,E10.3,15X,E10.3)	NUCREA	333
364 FORMAT (5X,19HENERGY/CHANNEL (KEV),10X,6HQ (KEV),20X,3HCON)	NUCREA	334
365 FORMAT (10X,E10.3,11X,E10.3,15X,E10.3)	NUCREA	335
366 FORMAT (5X,1HZ,10X,1HA,10X,2HEN,10X,11H1A,1H,4A,4B)	NUCREA	336
367 FORMAT (2X,3(E11.3))	NUCREA	337
368 FORMAT (5X,7HEN(KEV),10X,5HSIGMA,10X,14HCENTER OF MASS)	NUCREA	338
369 FORMAT (4X,E10.3,5X,E10.3)	NUCREA	339
370 FORMAT (5X,7HEN(KEV),10X,5HSIGMA,10X,3HLAB)	NUCREA	340
371 FORMAT (6X,1HI,7X,SHYIELD)	NUCREA	341
372 FORMAT (5X,2HZA,8X,2H2B)	NUCREA	342
END	NUCREA	343

SUBROUTINE SECALC(Z1,Z2,P1,E,SE,Z,A,N)	NUCREA	344
Z1,Z2 ARE THE ATOMIC NUMBERS OF THE INCIDENT ION AND TARGET RESPEC	NUCREA	345
P1 IS THE INCIDENT ION MASS IN AMU	NUCREA	346
E IS THE INCIDENT ENERGY IN KEV	NUCREA	347
SE IS THE INELASTIC STOPPING CROSS SECTION IN KEV-CM2/ATOM(MOLECUL	NUCREA	348
Z,A,N ARE THE THREE PARAMETERS Z,A,N,RESPECTIVELY	NUCREA	349
$\alpha = 1.21918E-18$	NUCREA	350
$X = E/(100.*P1)$	NUCREA	351
$Y = X/(Z**2)$	NUCREA	352
$SQ = \text{SQRT}(Y)$	NUCREA	353
$AT = \text{ATAN}(SQ)$	NUCREA	354
$SE = (((30.*Y+83.)*Y+74.)*Y+21.)$	NUCREA	355
$SE = SE/(3.*(1.+Y)**3)$	NUCREA	356
$SE = SE*SE+AT*(10.*Y+1.)$	NUCREA	357
$SE = H*SE$	NUCREA	358
$SE = SE*(Z1/Z2)/2.$	NUCREA	359
$SQ = 2.*\text{SQRT}(X)*A$	NUCREA	360
$Y = 1.+SQ**N$	NUCREA	361
$SE = SE/Y$	NUCREA	362
RETURN	NUCREA	363
END	NUCREA	364

VI. NUCREA: TYPICAL OUTPUT

The output listed in this section gives an analysis of the spectrum shown in Fig. 2. The analysis is discussed in more detail in Section III-B. The output consists of a printout of the input information followed by information generated in analysis of the spectrum. In addition, an output section is listed which gives the analysis of the spectrum shown in Fig. 2 for a 650-keV ^3He ion beam incident on a $\text{ScD}_{1.8}$ film on a kovar substrate. The computer graphical output is shown in Figs. 3 and 4; in Fig. 3 is shown the input spectrum and in Fig. 4 is shown the results of the calculation. The reader is reminded that no straggling effects or detector resolution or effects are included in the calculation.

Fig. 2 - Experimental Spectrum for 650 keV He^3 ions incident on a 0.21 mg/cm² ScD_2 film on a kovar substrate.

Fig. 3 - Graphical computer output of that part of spectrum shown in Fig. 2 which is analyzed. Data has been smoothed.

650 keV ^3He on $\text{ScD}_2/\text{Kovar}$

March 10, 1975, SPECTRA 4

Fig. 4 - Graphical computer output of analyzed spectrum. NB/NA is the ratio of the number of B atoms/cm³(D) to the number of A atoms/cm³(Sc).

650KEV HE3 ON SCD2/KOVAR MARCH 10, 1975 SPECTRA 4 (SMOOTHED DATA)

ANGLE OF ATTACK
1.571E+00

SCATTERING ANGLE
2.967E+00

Z1	Z2	Z3	Z4	M1	M2	M3	M4
2.0000	1.0000	1.0000	2.0000	3.0160	2.0140	1.0080	4.0030

ZA	ZB
21.0000	1.0000

ENERGY/CHANNEL (KEV)
4.860E+00

Q (KEV)
1.835E+04

CON
1.490E-11

Z	A	EM	1A,1B,4A,4B
1.398E+00	4.016E-01	3.343E+00	
1.202E+00	4.384E-01	3.683E+00	
1.398E+00	4.016E-01	3.343E+00	
1.202E+00	4.384E-01	3.683E+00	

1	YIELD
1	1.560E+02
2	2.690E+02
3	2.960E+02
4	3.500E+02
5	3.660E+02
6	3.680E+02
7	3.600E+02
8	3.500E+02
9	3.310E+02
10	3.070E+02
11	2.960E+02
12	2.820E+02
13	2.710E+02
14	2.570E+02
15	2.450E+02
16	2.320E+02
17	2.210E+02
18	2.120E+02
19	2.020E+02
20	1.950E+02
21	1.840E+02
22	1.750E+02
23	1.640E+02
24	1.550E+02
25	1.430E+02
26	1.350E+02
27	1.280E+02
28	1.220E+02
29	1.150E+02
30	1.070E+02
31	1.010E+02
32	9.600E+01
33	9.400E+01
34	9.300E+01
35	7.100E+01
36	6.500E+01
37	6.000E+01
38	5.500E+01
39	5.200E+01
40	4.800E+01
41	4.500E+01
42	4.000E+01
43	3.700E+01
44	3.400E+01
45	3.100E+01
46	2.700E+01
47	2.300E+01
48	2.000E+01
49	1.800E+01
50	1.500E+01

HE3(D,P)HE4 SIGMA FROM YARNELL ET AL. PHYS. REV. 90, 292 (1953)

EN (KEV)	SIGMA	CENTER OF MASS
3.570E+02	2.350E+01	
4.230E+02	3.680E+01	
4.800E+02	5.480E+01	
5.480E+02	6.500E+01	
5.700E+02	7.000E+01	
6.090E+02	6.950E+01	
6.410E+02	7.170E+01	
6.680E+02	7.150E+01	
7.100E+02	6.880E+01	
7.280E+02	6.630E+01	
7.580E+02	6.380E+01	
7.880E+02	5.980E+01	
8.480E+02	5.400E+01	
9.080E+02	4.830E+01	
1.017E+03	3.980E+01	
1.133E+03	3.300E+01	
1.245E+03	2.770E+01	
1.365E+03	2.470E+01	

EN (KEV)	SIGMA	LAB
3.570E+02	1.461E-26	
4.230E+02	2.181E-26	
4.800E+02	3.112E-26	
5.480E+02	3.543E-26	
5.700E+02	3.762E-26	
6.090E+02	3.646E-26	
6.410E+02	3.688E-26	
6.680E+02	3.618E-26	
7.100E+02	3.345E-26	
7.280E+02	3.238E-26	
7.580E+02	3.062E-26	
7.880E+02	2.821E-26	
8.480E+02	2.462E-26	
9.080E+02	2.130E-26	
1.017E+03	1.655E-26	
1.133E+03	1.291E-26	
1.245E+03	1.023E-26	
1.365E+03	8.591E-27	

P(1.1-43)										
1	.468	.463	.466	.469	.472	.475	.478	.482	.485	.488
2	.997	.914	.921	.928	.935	.942	.949	.957	.964	.972
3	1.047	1.105	1.115	1.124	1.133	1.141	1.150	1.159	1.168	1.176
4	1.659	1.670	1.680	1.690	1.691	1.511	1.520	1.530	1.539	1.548
5	1.661	1.670	1.679	1.687	1.695	1.703	1.710	1.718	1.725	1.732
6	1.739	1.745	1.752	1.759	1.765	1.772	1.778	1.785	1.791	1.793
7	1.753	1.760	1.767	1.774	1.781	1.788	1.796	1.804	1.812	1.820
8	1.762	1.771	1.780	1.789	1.799	1.809	1.820	1.831	1.842	1.854
9	1.733	1.745	1.758	1.770	1.783	1.797	1.811	1.825	1.840	1.855
10	1.693	1.706	1.720	1.734	1.749	1.763	1.778	1.792	1.807	1.822
11	1.750	1.764	1.778	1.792	1.806	1.820	1.833	1.847	1.860	1.874
12	1.769	1.782	1.796	1.810	1.818	1.830	1.841	1.853	1.865	1.876
13	1.790	1.801	1.812	1.822	1.833	1.843	1.854	1.864	1.875	1.885
14	1.766	1.776	1.785	1.794	1.804	1.813	1.822	1.832	1.841	1.850
15	1.745	1.754	1.763	1.771	1.780	1.789	1.797	1.806	1.815	1.823
16	1.705	1.713	1.721	1.729	1.738	1.746	1.754	1.763	1.771	1.779
17	1.677	1.685	1.693	1.702	1.710	1.718	1.726	1.735	1.743	1.752
18	1.667	1.676	1.684	1.692	1.701	1.710	1.718	1.727	1.736	1.745
19	1.647	1.656	1.665	1.674	1.683	1.692	1.702	1.711	1.721	1.731
20	1.652	1.672	1.682	1.692	1.702	1.712	1.723	1.734	1.745	1.756
21	1.638	1.648	1.659	1.670	1.681	1.692	1.703	1.715	1.727	1.739
22	1.640	1.651	1.663	1.674	1.686	1.698	1.711	1.723	1.736	1.748
23	1.613	1.630	1.642	1.654	1.666	1.679	1.692	1.704	1.718	1.731
24	1.620	1.633	1.645	1.658	1.671	1.684	1.697	1.710	1.724	1.737
25	1.677	1.689	1.699	1.614	1.627	1.640	1.653	1.666	1.679	1.693
26	1.684	1.696	1.699	1.622	1.635	1.648	1.661	1.674	1.688	1.701
27	1.600	1.613	1.625	1.639	1.652	1.665	1.679	1.692	1.706	1.719
28	1.628	1.641	1.654	1.667	1.680	1.693	1.706	1.720	1.733	1.747
29	1.630	1.642	1.655	1.667	1.680	1.693	1.706	1.719	1.732	1.745
30	1.600	1.612	1.624	1.635	1.647	1.659	1.671	1.683	1.695	1.707
31	1.695	1.696	1.617	1.629	1.640	1.651	1.663	1.674	1.685	1.697
32	1.699	1.610	1.621	1.631	1.642	1.653	1.664	1.675	1.686	1.697
33	1.661	1.672	1.683	1.693	1.704	1.715	1.726	1.737	1.748	1.759
34	1.765	1.785	1.797	1.777	1.788	1.799	1.810	1.822	1.833	1.844
35	1.311	1.318	1.326	1.333	1.341	1.348	1.356	1.363	1.371	1.378
36	1.262	1.269	1.266	1.263	1.269	1.276	1.283	1.290	1.297	1.303
37	1.193	1.194	1.200	1.206	1.212	1.219	1.225	1.231	1.237	1.244
38	1.124	1.130	1.136	1.141	1.147	1.153	1.158	1.164	1.170	1.176
39	1.109	1.112	1.115	1.120	1.125	1.131	1.136	1.142	1.147	1.153
40	1.052	1.057	1.062	1.067	1.072	1.077	1.082	1.087	1.092	1.098
41	1.021	1.025	1.030	1.035	1.040	1.045	1.050	1.055	1.059	1.064
42	.930	.934	.939	.943	.947	.952	.956	.960	.965	.969
43	.909	.913	.917	.921	.925	.929	.933	.937	.942	.946
44	.843	.847	.851	.854	.858	.862	.866	.870	.874	.878
45	.753	.757	.760	.764	.768	.771	.775	.779	.783	.787
46	.709	.713	.716	.719	.722	.726	.729	.733	.736	.740
47	.620	.623	.626	.629	.632	.635	.638	.641	.644	.647
48	.557	.560	.562	.565	.568	.570	.573	.576	.579	.582
49	.521	.523	.526	.528	.531	.534	.536	.539	.542	.545
50	.449	.451	.453	.456	.458	.460	.463	.465	.468	.470

CHANNEL	YIELD COUNT	EF KEV	EF KEV	DX A-ATOMS/CM2	X A-ATOMS/CM2	L A-ATOMS/CM2	NB/NA
1	155.00	5.587E+02	1.900E+03	1.336E+17	1.336E+17	1.336E+17	4.739E-01
2	269.00	5.450E+02	1.495E+03	1.159E+17	2.496E+17	2.496E+17	9.387E-01
3	295.00	5.323E+02	1.710E+03	1.060E+17	3.556E+17	3.556E+17	1.137E+00
4	350.00	5.204E+02	1.915E+03	9.518E+16	4.508E+17	4.508E+17	1.505E+00
5	354.00	5.092E+02	1.919E+03	8.821E+16	5.390E+17	5.390E+17	1.698E+00
6	368.00	5.986E+02	1.924E+03	8.349E+16	6.225E+17	6.225E+17	1.768E+00
7	360.00	5.884E+02	1.929E+03	7.986E+16	7.023E+17	7.023E+17	1.786E+00
8	350.00	5.785E+02	1.934E+03	7.655E+16	7.789E+17	7.789E+17	1.806E+00
9	331.00	5.692E+02	1.939E+03	7.388E+16	8.527E+17	8.527E+17	1.792E+00
10	307.00	5.602E+02	1.944E+03	7.166E+16	9.244E+17	9.244E+17	1.757E+00
11	296.00	5.514E+02	1.949E+03	6.877E+16	9.932E+17	9.932E+17	1.813E+00
12	282.00	5.429E+02	1.953E+03	6.652E+16	1.060E+18	1.060E+18	1.823E+00
13	271.00	5.347E+02	1.958E+03	6.440E+16	1.124E+18	1.124E+18	1.838E+00
14	257.00	5.267E+02	1.963E+03	6.281E+16	1.187E+18	1.187E+18	1.808E+00
15	245.00	5.189E+02	1.968E+03	6.129E+16	1.248E+18	1.248E+18	1.784E+00
16	232.00	5.114E+02	1.973E+03	6.002E+16	1.308E+18	1.308E+18	1.742E+00
17	221.00	5.040E+02	1.978E+03	5.872E+16	1.367E+18	1.367E+18	1.714E+00
18	212.00	4.968E+02	1.983E+03	5.736E+16	1.424E+18	1.424E+18	1.706E+00
19	202.00	4.897E+02	1.987E+03	5.615E+16	1.480E+18	1.480E+18	1.688E+00
20	195.00	4.829E+02	1.992E+03	5.473E+16	1.535E+18	1.535E+18	1.708E+00
21	184.00	4.761E+02	1.997E+03	5.369E+16	1.589E+18	1.589E+18	1.687E+00
22	175.00	4.696E+02	2.002E+03	5.251E+16	1.641E+18	1.641E+18	1.693E+00
23	164.00	4.631E+02	2.007E+03	5.158E+16	1.693E+18	1.693E+18	1.673E+00
24	155.00	4.568E+02	2.012E+03	5.052E+16	1.743E+18	1.743E+18	1.678E+00
25	143.00	4.506E+02	2.017E+03	4.986E+16	1.793E+18	1.793E+18	1.634E+00
26	135.00	4.446E+02	2.021E+03	4.888E+16	1.842E+18	1.842E+18	1.642E+00
27	128.00	4.386E+02	2.026E+03	4.788E+16	1.890E+18	1.890E+18	1.659E+00
28	122.00	4.328E+02	2.031E+03	4.686E+16	1.937E+18	1.937E+18	1.687E+00
29	115.00	4.271E+02	2.036E+03	4.606E+16	1.983E+18	1.983E+18	1.687E+00
30	107.00	4.215E+02	2.041E+03	4.551E+16	2.029E+18	2.029E+18	1.653E+00
31	101.00	4.159E+02	2.046E+03	4.483E+16	2.073E+18	2.073E+18	1.646E+00
32	96.00	4.105E+02	2.051E+03	4.412E+16	2.117E+18	2.117E+18	1.648E+00
33	94.00	4.052E+02	2.056E+03	4.307E+16	2.161E+18	2.161E+18	1.710E+00
34	93.00	3.999E+02	2.060E+03	4.194E+16	2.202E+18	2.202E+18	1.794E+00
35	71.00	3.948E+02	2.065E+03	4.406E+16	2.247E+18	2.247E+18	1.345E+00
36	65.00	3.896E+02	2.070E+03	4.390E+16	2.290E+18	2.290E+18	1.273E+00
37	50.00	3.846E+02	2.075E+03	4.367E+16	2.334E+18	2.334E+18	1.216E+00
38	55.00	3.796E+02	2.080E+03	4.351E+16	2.378E+18	2.378E+18	1.150E+00
39	52.00	3.747E+02	2.085E+03	4.308E+16	2.421E+18	2.421E+18	1.128E+00
40	48.00	3.699E+02	2.090E+03	4.288E+16	2.464E+18	2.464E+18	1.075E+00
41	45.00	3.651E+02	2.094E+03	4.255E+16	2.506E+18	2.506E+18	1.042E+00
42	49.00	3.604E+02	2.099E+03	4.264E+16	2.549E+18	2.549E+18	9.496E-01
43	37.00	3.558E+02	2.104E+03	4.242E+16	2.591E+18	2.591E+18	9.071E-01
44	34.00	3.512E+02	2.109E+03	4.224E+16	2.633E+18	2.633E+18	8.604E-01
45	31.00	3.467E+02	2.114E+03	4.210E+16	2.676E+18	2.676E+18	8.097E-01
46	27.00	3.422E+02	2.119E+03	4.221E+16	2.718E+18	2.718E+18	7.243E-01
47	23.00	3.375E+02	2.124E+03	4.238E+16	2.760E+18	2.760E+18	6.337E-01
48	20.00	3.334E+02	2.129E+03	4.238E+16	2.802E+18	2.802E+18	5.692E-01
49	18.00	3.291E+02	2.133E+03	4.220E+16	2.845E+18	2.845E+18	5.325E-01
50	15.00	3.248E+02	2.137E+03	4.230E+16	2.887E+18	2.887E+18	4.593E-01

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