22
3-1-79
24 to 7/1/8
MASTER

**Analysis of a Nuclear Backscattering
and Reaction Data by the Method
of Convolution Integrals**

M. B. Lewis

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION • FOR THE DEPARTMENT OF ENERGY

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
Price: Printed Copy \$4.50; Microfiche \$3.00

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, contractors, subcontractors, or their employees, makes any warranty, express or implied, nor assumes any legal liability or responsibility for any third party's use or the results of such use of any information, apparatus, product or process disclosed in this report, nor represents that its use by such third party would not infringe privately owned rights.

Contract No. W-7405-eng-26

METALS AND CERAMICS DIVISION

ANALYSIS OF A NUCLEAR BACKSCATTERING AND REACTION DATA
BY THE METHOD OF CONVOLUTION INTEGRALS

M. B. Lewis

Date Published - February 1979

NOTICE This document contains information of a preliminary nature.
It is subject to revision or correction and therefore does not represent a
final report.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

NOTICE
This report was prepared as an account of work
sponsored by the United States Government. Neither the
United States nor the United States Department of
Energy, nor any of their employees, nor any of their
contractors, subcontractors, or their employees, makes
any warranty, express or implied, or assumes any legal
liability or responsibility for the accuracy, completeness
or usefulness of any information, apparatus, product or
process disclosed, or represents that its use would not
infringe privately owned rights.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

CONTENTS

INTRODUCTION	1
METHOD	3
APPLICATIONS	11
SUMMARY	16
REFERENCES	16
APPENDIX	17
A. Definitions of mathematical symbols	17
B. Formulas and Approximations.	18
C. Convolution Integrals	21
D. Numerical Approximation	21
E. Input Format for BASS	24
F. Listing of BASS	25

ANALYSIS OF A NUCLEAR BACKSCATTERING AND REACTION DATA
BY THE METHOD OF CONVOLUTION INTEGRALS

M. B. Lewis

ABSTRACT

A quantitative description of nuclear backscattering and reaction processes has been made. Various formulas pertinent to nuclear microanalysis have been assembled in a manner useful for experimental application. Convolution integrals relating profiles of atoms in a metal substrate to the nuclear reaction spectra obtained in the laboratory have been described and computed. Energy straggling and multiple scattering have been explicitly included and shown to be important. Examples of the application of the method to simple backscattering, oxide films and implanted gas have been discussed.

INTRODUCTION

When an atomic ion beam impinges on a target, the ions traverse an almost straight path into the material, gradually losing energy by atomic excitation of the host electrons. Occasionally, however, an individual ion makes a sufficiently close approach to a target nucleus that the ion is deflected by the coulomb electric field between the nuclei. In some deflections the incident ions may reappear from the target surface. Such processes are referred to as elastic "backscattering." Less frequently, but to a measurable extent, the distance of closest approach of the nuclei may be such that their nuclear fields interact and a nuclear transmutation occurs. If one of the products of this reaction is emitted from the target surface, the process is referred to nuclear reaction "backscattering." During the past thirty years these nuclear reactions have been rather extensively characterized. In addition, the energy loss rate of

ions in pure materials has been measured. For these reasons, it has more recently been demonstrated that the process of ion (elastic and nuclear reaction) backscattering is a valuable analytical tool for measuring the atomic components in a complex target.

As an example, refer to the schematic drawing in Fig. 1. Suppose that an unknown concentration of previously implanted foreign atoms $\rho(x)$ exists in a pure metal target host or substrate. Let x be the depth below the surface measured along the surface normal (i.e., projected depth). In the experiment, one allows an ion beam of measured energy and intensity to be incident on the target surface. The ions penetrate the material, occasionally "backscattering" and reappearing as a reaction ion. The energy spectrum or yield, $Y(E)$, of backscattered ions can be accurately measured. These ions may have the same mass as the incident ions (elastic scattering) or they may be new products

Fig. 1. Schematic Illustration of Ion Beam and Target Geometry Showing a Target Previously Implanted with Atomic Density ρ in a Target Substrate or Host.

(reaction scattering). This must be determined experimentally or by a general knowledge of nuclear reactions. Once the particular reaction has been identified, the energy of the reaction ion depends upon the path in the substrate which is traversed by the incident ion before the nuclear collision and the "backscattered" or reaction ion path after collision. For example, the further below the surface the collision takes place, usually the lower will be the reaction ion energy. For this reason the yield $Y(E)$ spectrum of backscattered ions implies a specific density distribution $\rho(x)$ depth profile of foreign atoms in the substrate. The purpose of this report is to demonstrate a method of calculating the function $Y(E)$ for a given density $\rho(x)$ by combining known properties of atomic and nuclear scattering.

METHOD

The basic approach to the convolution integral problem that we use here was suggested by Brice.¹ The target-beam geometry is shown in Fig. 2 where the shaded area refers to the target host or substrate in which an unknown density of foreign atoms resides. A summary of the frequently used symbols and their definitions can be found in Appendix A. The method assumes that the probability, Y , of measuring a reaction ion of energy E_r at a backscattering angle θ is equal to the probability, I , that an incident ion exists in the substrate times the probability, ρ , that a foreign atom exist in substrate times the probability σ that the proper nuclear event will occur times the probability, R , that the desired reaction ion will be emitted at the target surface and detected with energy E_r at angle θ ; symbolically we have

$$Y = Ip\sigma R \quad (1)$$

Our particular computational approach is outlined in six basic steps shown in Fig. 3. In Eq. (1), I and R are computed below in Section 5.

ORNL-DWG 78-46028

Fig. 2. Detailed View of Ion-Target Geometry for Arbitrary Target Orientation.

ORNL-DWG 78-2762R

SPECTRUM SIMULATION

1. $S(E) = \sum_n a_n E^n$ INTERPOLATION (FOR i AND r)
2. $(\Delta E_i)_{x_j} = \int_0^{x_i} S_i(E_i) dx$ BY ITERATION
3. $(\Delta E_r)_{x_j} = \int_{x_j}^0 S_r(K(E_i, \theta)) dx$ BY ITERATION
4. $\sigma(E_i) = \sum_m b_m E_i^m$ INTERPOLATION (FOR GIVEN θ)
5. $P(E, \bar{E}, x) =$ GAUSSIAN PROBABILITY DISTRIBUTION FOR i AND r
6. $Y(E_r)/\Delta E_r =$ CONVOLUTION OF 4 AND 5 WITH SELECTED DENSITY ρ PROFILE

$$= \int_0^\infty c\rho(x)dx \int_0^\infty P_i(E, \bar{E}_i, x) \sigma(E) P_r(E, \bar{E}_r, x) dE$$

Fig. 3. Outline of Basic Steps used to Calculate a Backangle Spectrum of Ion Yield vs Energy.

1. S(E) Since the nuclear cross section σ is dependent upon the energy of the incident ion $E_i(x)$ below the target surface, this energy must be estimated as a function of x . The ion stopping power $S(E)$ is required. A recent data evaluation² of hydrogen and helium stopping powers makes it possible to select a few values which are relevant to a particular case. If the target substrate is complex or if the density of foreign atoms is large, the so-called Bragg rule approximation³ is made so the effective stopping power is

$$S_{\text{eff}} = \sum_j S_j \rho_j \quad (2)$$

where S_j is the stopping power (ev/atom/cm²) of type j and ρ_j is its atomic density (atom/cm³) in the complex target. The computation proceeds by making a third order polynomial least squares fit to selected values of S for both the incident ion and reaction ion. This yields a simple analytical function $S(E)$ over the region of interest.

2. $(\Delta E_i)_{x_j}$ The depth region is now divided into 100 differential slices Δx so that $x = x_j = j\Delta x$ where $j = 1, 2, \dots, 100$ (see Fig. 2). The mean energy loss

$$(\Delta E_i)_{x_j} = \sum_{k=1}^j S_i(E_k) \Delta x_k \quad (3)$$

can be made by iteration beginning at the target surface. When complete we have an energy dependence of the ion as a function of depth by

$$E_i(x_j) = E_i(0) - (\Delta E_i)_{x_j} \quad (4)$$

3. $(\Delta E_r)_{x_j}$ At the depth x_j a nuclear reaction is assumed to occur. The relation $E_r = KE_i$ between the energy of the incident ion and reaction ion is given by classical kinematics⁴

$$(E_r)^{1/2} = v \pm (v^2 + w)^{1/2} \quad (5)$$

where

$$v = (M_i M_r E_i)^{1/2} \cos\theta / (M_r + M_4)$$

$$w = (M_4 Q + E_i (M_4 - M_i)) / (M_r + M_4)$$

M_4 = residual mass

Q = mass-energy excess.

The energy of the reaction ion as it emerges from the target surface is then

$$E_r(0) = E_r - (\Delta E_r)_{x_j} \quad (6)$$

in which the iteration is now reversed and begins below the surface at x_j . When complete we now have the mean energy of reaction ions as a function of the depth below the surface at which a nuclear event took place.

4. $\sigma(E_i)$ The nuclear cross section for elastic scattering is analytical^{3,4}

$$\sigma_{lab}(E_i) = b^2/16 [\sin^4(\theta/2) - 2(M_i/M_2)^2] \quad (7)$$

where $b = Z_i Z_2 e^2 / E_i$ is the distance of closest approach between the ions, or expressing E in MeV and σ in millibarns/steradian

$$\sigma_{lab}(E_i) = 1.295 (Z_i Z_2 / E_i)^2 [\csc^4(\theta/2) - 2(M_i/M_2)^2] .$$

However, in the case of nuclear reaction events one usually obtains from the literature only a few values of σ at discrete energies. For this reason it is necessary to interpolate. This is carried out by an n^{th} order polynomial least squares fit through the selected values in the energy region of interest. Where necessary the values of σ are transformed to the laboratory coordinate system⁵ so that the final computation for $Y(E)$ can be directly compared to raw data.

5. $P(E, \bar{E}, X)$ As the ion traverses a finite path in the target, it makes a finite number of collisions with electrons, and independently,

a finite number of collisions with nuclei at random intervals of time between collisions for each process. If $\bar{n}$ is the average number of any type of collision along a certain path then the standard deviation of such events is $\Omega = (\bar{n})^{1/2}$, and the statistical distribution is given by⁴

$$P(n) = (2\pi)^{-1/2} \Omega^{-1} \exp[-(n - \bar{n})^2 / 2\Omega^2] \quad (8)$$

where $P(n)$ is the probability that n collisions will take place along the path.

Each ion collision with an electron results in a small ion energy loss (approximately the electron binding energy) and the average number of such collisions is determined approximately by the linear density of electrons times the path length. Based on these ideas Bohr⁶ suggested a formula for energy "straggling" or uncertainty for path length X ,

$$\Omega_i^2(x) = 4\pi e^4 X Z_i^2 Z_2 \rho \quad (9a)$$

where Z_i , Z_2 , and ρ are the ion atomic number, target atomic number and target atomic density. Assuming chemical potential effects are not important, straggling in a complex target would be estimated by the statistical sum

$$\Omega_{\text{eff}}^2 = \sum_{j=1}^n \Omega_j^2 = 4\pi e^4 X Z_i^2 \sum_{j=1}^n Z_2 \rho_j \quad (9b)$$

where ρ_j is the elemental atomic density and n the number of target constituents. In practice an effective ρ_{eff} can be used such that

$$Z \rho_{\text{eff}} = \sum_{j=1}^n Z_2 \rho_j$$

where Z is an arbitrary target element number chosen to satisfy the effective charge in multiple scattering [see Eq. (14b)]. It is well known,³ however, that the Bohr treatment is incomplete for at least

two reasons: (a) the ion has a finite probability of absorbing electrons as it slows down to velocities v comparable to electron orbital velocities v_0

$$v_0 \approx e^2/h . \quad (10)$$

This reduces the effective charge of the ion and therefore the straggling. (b) The binding energy of an electron is subject to "shell" or quantum effects which cannot be expressed in simple analytic form. Our computational method is to use the Bohr approximation, but to make small corrections to the ion charge Z_i if warranted by direct measurements of ion straggling in the energy and mass region of interest. In addition to the straggling, the incident ion energy is uncertain due to the finite resolution $\Omega_i(0)$ with which one can measure the accelerated ion energy. If we assume that this uncertainty also follows a Gaussian distribution, we can then combine the uncertainties into a total width

$$\Omega_i^2 = \Omega_i^2(0) + \Omega_i^2(x) \quad (11)$$

This depth dependent straggling and mean energy $\bar{E}_i(x)$ (see procedure 3) define the incident ion probability density [I in Eq. (1)]

$$I = P(E_i, \bar{E}_i, x) = (2\pi)^{-1/2} \Omega_i^{-1} \exp[-(E - \bar{E}_i)^2 / 2\Omega_i^2] . \quad (12)$$

In a similar way we calculate the reaction probability density by estimating Ω_r as a function of depth x . However, as shown below additional factors appear which contribute to Ω .

Each ion collision with a nucleus scatters the ion slightly off axis from its mean direction. This implies that for backscattering events occurring below the target surface, the incident angle α_i is not unique but has a statistical deviation. Moliere⁷ calculated this deviation. Dickinson and Dodder⁸ suggest a useful approximation of Moliere's expression to be

$$(\Delta\alpha_i)^2 = \frac{BZ_2 \ln(E_{in}/E_{out})}{4(M_i/m) \ln(297\beta/Z_2^{1/2})} \quad (13)$$

where B is the number of collisions, E_{in}/E_{out} is the ratio of ion energy before and after passing through a foil, m is the mass of an electron and β is the ratio of the ion velocity to the velocity of light. For ions of relatively low energy and heavy mass Meyer⁹ has shown the Moliere's theory needs to be modified for targets of small thickness. Reevaluation of Meyer's calculations have also been made by Sigmund and Winterbon.¹⁰ In the present calculations we use an approximation suggested by Cohen¹¹ for light ions in the low MeV energy region:

$$(\Delta\alpha_i)^2 = \frac{Z_2(E_{in} - E_{out})}{(M_i/m)\bar{E}} \text{ radians} \quad (14)$$

where $\bar{E}$ is the average energy of the ion in the foil. The usefulness of this relatively simple form is illustrated by comparing its values with those of the more complex forms of Moliere and Meyer shown in Table 1. In the examples, the values of Moliere were taken from Ref. 12 while those based on Meyer are from Ref. 13.

Table 1. Comparison of Numerical Values of the r.m.s. Angular Spread of Deuterium Ions Penetrating Solid Targets.
The Calculations Which were Based Upon Theories of Multiple Scattering are Further Discussed in the Text.

Target	Thick (mg/cm ²)	E _{ion} (MeV)	$\Delta\alpha$ (deg)	Reference
Copper	1.0	5.0	0.63	11
			0.64	12
Uranium	0.16	0.3	1.86	11
			1.78	13

In Moliere's solution the multiple scattering is proportional to $Z_2^2 \rho$, analogous to Eq. (9). For a complex target, the effective charge Z for multiple scattering [analogous to Eq. (9b)] is written

$$Z^2 \rho_{\text{eff}} = \sum Z_{2j}^2 \rho_j . \quad (14b)$$

Dividing Eq. (14b) by Eq. (9b) we get

$$Z = \sum Z_{2j}^2 \rho_j / \sum Z_{2j}^2 \rho_j . \quad (14c)$$

Multiple scattering implies that the transmission probability of an ion through a foil is less than unity. Only in some experiments is this a problem, and convenient graphs exist for estimating losses.¹¹ Since the value of the reaction ion energy depends upon the incident ion angle, the uncertainty $\Delta\alpha_i$ in the incident ion angle implies an uncertainty in the reaction ion energy according to

$$(\Delta E_r)_{\Delta\alpha_i} = \frac{dE_r}{d\alpha_i} \Delta\alpha_i . \quad (15)$$

The reaction ion energy is measured by a detector which subtends a finite solid angle with the target beam spot. In the plane defined by the incident and reaction ion momenta the angular opening, $\Delta\alpha_r$, in the detector implies an uncertainty in reaction ion energy according to

$$(\Delta E_r)_{\Delta\alpha_r} = \frac{dE_r}{d\alpha_r} \Delta\alpha_r . \quad (16)$$

Finally, the detector system has finite resolution Ω_d which can be independently determined. As an approximation we combine these three components statistically along with the reaction ion straggling $\Omega_r(x)$ analogous to the incident ion case (Eq. 9)

$$\Omega_r^2 = (\Delta E_r)_{\Delta\alpha_i}^2 + (\Delta E_r)_{\Delta\alpha_r}^2 + \Omega_d^2 + \Omega_r^2(x) . \quad (17)$$

This value of Ω_r and the mean energy $\bar{E}_r$ previously estimated determine the reaction ion probability density, R in Eq. (1).

6. $Y(E_r)/\Delta E_r$ We have now computed the four functions symbolically given in Eq. (1). It remains to choose a profile density ρ and to integrate these over all physical and energy space in order to get a total probability. Since the measurement of reactions takes place in discrete and differential energy ΔE_r units called "channels" it is not required to integrate over E_r space other than the channel width ΔE_r . Also the target is assumed to be isotropic in the y-z plane (i.e., its surface). Therefore, we need only to compute the convolution integral over the energy range of the incident ion and the depth range of the ion in the target.

$$Y(E_r) = C \int \rho dx / P_i \sigma P_r dE_i \Delta E_r . \quad (18)$$

The value of the constant C depends upon the number of incident ions and the solid angle of the target according to the definition of a cross section.

$$\sigma(\theta) = \frac{\text{scattered ions/solid angle}}{\text{incident ions/area}} . \quad (19)$$

APPLICATIONS

Appendices B and C summarize the formulas and Appendix D the basic steps used in the computer calculations. Appendix E is a listing of the "Back-Angle Spectrum Simulation" code BASS.

The first application of the code is to calculate an elastic backscattering spectrum for a simple uniform target. An example is illustrated in Fig. 4 along with a measured spectrum for the $^{58}\text{Ni}(d,d)$ reaction. The characteristic features of the experimental spectrum which are properly simulated by the code are (a) the very slightly increasing yield (counts/channel) in the lower 100 channels (reaction ion energy) which is expected from the inverse energy dependence of the elastic cross section [see Eq. (7)], and (b) the exponential

Fig. 4. Example of Backangle Spectrum from Deuterons Elastically Scattered from a Nickel Target. A calculated curve is also shown.

decrease in yield in the maximum energy region (channels 600–620) which reflects the statistical nature of energy straggling and detector resolution for ions scattered from the near surface region of the target. The normalization of the computed curve in Fig. 4 is adjusted within the uncertainty of the measured values of counts per channel ($\approx 10\%$) and channel number ($\approx 3\%$).

A different application of the simulation method is to determine the density profile of helium (^3He) and hydrogen (^2H) which had been implanted in a nickel substrate. The calculated curve and data are shown in Fig. 5. The curve for the $^3\text{He} (d, \alpha)$ reaction is seen to be considerably broader than that for the $^2\text{H} (d, p)$ reaction. The data are properly simulated by the calculated curves owing to the much larger stopping power and energy loss for the reaction ion alpha (α) particles compared to protons (p). The values of mean depth x_0 and standard deviation σ for the helium distribution are also accurately deduced from the fit to the data when a Gaussian density profile is assumed for $\rho(x)$.

Fig. 5. Example of a Backangle Reaction Spectrum in which Helium and Hydrogen (Deuterium) are Profiled in a Nickel Substrate. Edge refers to the spectral region where hydrogen or helium on the surface edge of the target would yield counts. Also given are the center and width of the Gaussian function (He profile) used to calculate the convolution integrals for the He curve.

As another illustration we apply the code to deduce the widths of oxide films on targets of vanadium and zirconium. The data for the $^{16}\text{O}(d,p)$ and $^{18}\text{O}(p,\alpha)$ reactions are shown in Fig. 6. Although the films are uniform in their oxygen density, the data show distinct slopes along the tops of the peaks. The calculated curve reproduces this effect, and its origin is the strong energy dependence of the reaction cross section at low bombardment energies (≈ 0.45 MeV).

The sensitivity of the nuclear microanalysis technique is strongly dependent upon the particular application. For example, the application which utilizes the maximum sensitivity of this technique is the measurement of a thin film of a high atomic number element deposited on a lower atomic number substrate. Let us take the case of a uranium film deposited on stainless steel. From the formula in Appendix 1.4 and 4.3,

Fig. 6. Example of a Backangle Reaction Spectrum in which the Oxide Layer on Vanadium and Zirconium is Profiled with incident hydrogen beams.

we find that we could get a peak of about 100 counts in a 10 msr detector at the 170° backangle alpha spectrum in 60 min for a 1 MeV α -beam current of $0.1 \mu\text{A}$ ($100 \mu\text{C}$) on a uranium film of only $1/20,000$ of a monolayer. However, to get 100 counts from the oxygen-18 atoms on the same surface, we need $1/20$ monolayer as a target using the $^{18}\text{O}(p, \alpha)$ reaction.

In general, the depth resolution is limited by the uncertainties in the tabulated stopping powers. This means that a marker below the target surface cannot be measured with an uncertainty of less than about 5% of the depth below the surface. When the target is rotated to intercept the ions at an angle different from the normal, this depth uncertainty may decrease, but straggling and multiple scattering increases. If this technique is used in conjunction with target sputtering, depth resolution can sometimes be maximized. Without sputtering it is not usually possible to

locate markers in the 1st 100 Å below the surface due to finite detector resolution. However, since the nuclear microanalysis techniques are quantitative, the mass of a film can be measured with an accuracy of 5–15% independent of its depth or thickness. For lateral resolution, ion beam techniques are generally not competitive with electron techniques due to the difficulty of constructing an ion source with a very small diameter. The volume sensitivity, like the surface sensitivity, is very high when the representative peaks are isolated. If the uranium film discussed above were diffused throughout a depth of about 1000 Å, the volume sensitivity of the backscattering technique might be as high as 1/20 ppm. The most favorable nuclear reaction techniques such as $^{18}\text{O}(\text{p},\alpha)$ or $^3\text{He}(\text{d},\text{p})$ would have sensitivities of approximately 50 ppm for oxygen-18 and helium-3.

As a final example of sensitivity, we show in Fig. 7 a comparison of two depth profiles for the reaction indicated. Both calculations assume a Gaussian profile but with one standard deviation larger than the other. The resulting curves are sufficiently different in the region near channel 430 that the data can define the width (σ) of the profile to within about 10% of the total or ± 100 Å in this case. This

Fig. 7. Reaction Spectrum of Helium in which Two Computed Curves are Compared to the Data.

"spatial" resolution is limited primarily by the counting statistics of the data itself rather than the uncertainties in the stopping powers which limit the "depth" resolution discussed above.

SUMMARY

We have explained the nature of elastic reaction and backscattering spectra of moderate energy ions on complex targets. A computer code has been written as an aid in the determination of profiles of elemental matter hosted in a known substrate material. When an approximate profile is read into the code, the output, calculated by the convolution integral method, can be directly compared with experimental data. The profile can then be adjusted to fit the data accurately. Four illustrations of the use of the method have been presented. The illustrations show that backscattering data could be incorrectly interpreted without the application of the computational method.

REFERENCES

1. D. K. Brice, *Thin Solid Films*, 19: 121 (1973).
2. J. F. Ziegler, editor, *The Stopping and Ranges of Ions in Matter*, Vol. 3, 4, Pergamon Press, New York, 1977.
3. W. K. Chu, *Ion Beam Handbook for Material Analysis*, J. W. Mayer and E. Rimini, eds, Academic Press, New York (1977) p.2.
4. R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1955.
5. J. B. Marion, *Nuclear Data Tables*, 1960.
6. N. Bohr, *Phil. Mag.* 30: 581 (1915).
7. G. Moliere, *Z. Naturf* 3a: 78 (1948).
8. W. C. Dickinson and D. C. Dodder, *Rev. Sci. Inst.* 24: 428 (1952).
9. L. Meycr, *Physo. Stat. Sol.* 44: 253 (1971).
10. P. Sigmund and K. B. Winterbon, *Nucl. Inst. Meth.* 119: 541 (1974).
11. B. L. Cohen, *Rev. Sci. Inst.* 33: 85 (1962).
12. J. B. Ball, ORNL-3311 (1962).
13. R. O. Sayer, ORNL/CSD/TM/2 (1976).

APPENDIX

Simulation of Back-Scattering Spectra

A. Definitions of mathematical symbols (see also Fig. 2).

X	. . .	depth below target surface (projected)
$E_i(X)$	. .	incident ion energy at position X
M_i	. . .	incident ion mass
Z_i	. . .	incident ion atomic number
α_i	. . .	angle between the incident ion and the normal to target surface
$S_i(X)$	. .	stopping power of incident ion at position X
Q	. . .	energy excess released in the nuclear reaction between the incident ions and atoms implanted in the target
$E_r(X)$	. .	reaction ion energy at position X
M_r	. . .	reaction ion mass
Z_r	. . .	reaction ion atomic number
α_r	. . .	angle between the reaction ion and the normal to target surface
$S_r(X)$	. .	stopping power of reaction ion at position X
θ	. . .	angle between incident and reaction ions ($\pi - \theta = \alpha_i + \alpha_r$)
$\rho(X)$	. .	density of implanted ions at position X
$\sigma[E_i(X), \theta]$		nuclear cross section between the incident ion and implanted ion at position X for a given value θ
$Y(E_r)$	. .	yield of reaction ions having energy about E_r
N, T	. . .	substrate density, thickness
Z	. . .	substrate atomic number
$\Omega_i(0)$	. .	standard deviation of incident ion energy
Ω_d	. . .	energy resolution of reaction ion detector (FWHM = $2.36 \Omega_d$)
2,4	. . .	subscripts referring to target, residual nucleus in a nuclear reaction

B. Formulas and Approximations

1.0 Gaussian distribution about X_0 with standard deviation σ

$$G(X) = (2\pi)^{-1/2} \sigma^{-1} \exp[-(X - X_0)^2 / 2\sigma^2]$$

1.10 The energy straggling Ω of monoenergetic ions after traversing a path length x in a target follows a Gaussian distribution with standard deviation according to Bohr:

$$\Omega^2 = 4\pi e^4 x Z_1^2 Z \rho$$

where Z_1 , Z , and ρ are the ion atomic number, target atomic number and target (charge center) density. For a multiple component target of uniform composition

$$\Omega^2 = \sum_j \Omega_j^2 = 4\pi e^4 x Z_1^2 \sum_j Z_j \rho_j$$

1.11 The multiple scattering of intermediate energy ions after passing through a target, losing energy ΔE , causes an angular dispersion

$$(\Delta\alpha_1)^2 = Z_2 \Delta E / (M_1 / m) E_{av}$$

1.2 Peak concentration of implanted ions (charge = 1) in a substrate assuming a Gaussian distribution:

$$C_m = \frac{(4.13E - 6)QM}{\rho\sigma a} \text{ at. \%} = \frac{(2.49 E 16)Q}{\sigma a} \text{ atoms/cm}^3$$

where $Q(\mu C)$ is the charge accumulated over a beam area $a(\text{cm}^2)$ on target of density $\rho(\text{g/cm}^3)$ and mass M (amu). The standard deviation of the distribution is $\sigma(\mu m)$.

1.3 Total target of implanted ions after a charge accumulation of $Q(\mu C)$:

$$\tau = \frac{(1.04 \times 10^{-8}) Q m}{a} \text{ mg/cm}^2 = \frac{(6.24 \times 10^{12}) Q}{a} \text{ atoms/cm}^2$$

where $a(\text{cm}^2)$ the beam area and $m(\text{amu})$ the atomic mass of the implanted ion.

The relation between peak density and thickness is:

$$C_m (\text{at./cm}^3) = \frac{(1 \times 10^4) \tau (\text{at./cm}^2)}{\sqrt{2\pi} \sigma (\mu\text{m})} = 3989 \frac{\tau (\text{at./cm}^2)}{\sigma (\mu\text{m})}$$

- 1.4 Counts accumulated in the detector whose solid angle to target is $\Omega(\text{mb/sr})$ following a reaction with cross section $\sigma(\text{mb/sr})$:

$$C = 3760 Q \tau \Omega \sigma / m \text{ counts}$$

where $Q (\mu\text{C})$ is the accumulated charge on target of thickness $\tau(\text{mg/cm}^2)$ and mass $m (\text{amu})$.

- 2.1 Gaussian approximation for the energy distribution of the incident beam:

$$P(E) = (2\pi)^{-1/2} \Omega_b^{-1}(0) \exp[-(E - E_i(0))^2 / 2\Omega_b^2(0)]$$

where Ω_b = standard deviation assumed for the incident beam energy $E_i(0)$

- 3.1 Addition of standard deviations:

$$(a) \quad \Omega_i^2(X) = \Omega_b^2(0) + \Omega_{\text{ion}}^2(X) \text{ for the incident}$$

$$(b) \quad \Omega_r^2(X) = \Omega_d^2 + \Omega_{\text{ion}}^2(X) \text{ for the reaction ion}$$

where Ω_d is the resolution (FWHM/2.36) of the reaction ion detector.

- 4.1 Linear path for incident and reaction ions in the substrate so that

$$\bar{E}_i(X) = \bar{E}_i(0) - \int_0^{R_i} S_i(R) dR$$

$$\bar{E}_r(0) = \bar{E}_r(X) - \int_0^{R_r} S_r(R) dR$$

where

$$R_i = X/\cos \alpha_i \text{ and } R_r = X/\cos \alpha_r$$

The target has uniform composition and Bragg's rule is assumed if the composition is multiple:

$$S = \sum_j S_j \rho_j$$

where S_j is the elemental stopping power (eV/atoms/cm²) of type j and ρ_j is its target density (atoms/cm³)

4.2 The relation between the reaction and incident ion energy

$$(E_r)^{1/2} = v \pm (v^2 + w)^{1/2}$$

where

$$v = (M_i M_r E_i)^{1/2} \cos \theta / (M_r + M_t)$$

$$w = [M_t Q + E_i (M_t - M_i)] / (M_r + M_t)$$

Q = mass-energy excess

4.3 Elastic scattering cross section in lab coordinates

$$\sigma_L(E_i) = 1.295 (Z_1 Z_2 / E_i)^2 [\operatorname{cosec}^4(\theta/2) - 2(M_i/M_2)^2]$$

where σ units are mb/sr if E_i is MeV

C. Convolution Integrals

1. Probability that an incident ion from a beam of average energy $\bar{E}_i(0)$ with energy $E \pm \frac{1}{2} \Delta E$ will be found at position X .

$P_i(E, \bar{E}_i, X) \Delta E$ where P is the function given by B - 1, and $\bar{E}_i = \bar{E}_i(X)$ is given by B - 4.

2. Probability that a nuclear event will take place at $X \pm \frac{1}{2} \Delta X$.

$$\int P_i(E, \bar{E}_i, X) \sigma(E) \rho(X) dE \Delta X.$$

3. Probability that after a nuclear event at $X \pm \frac{1}{2} \Delta X$, the reaction will have energy $E_r(0) \pm \frac{1}{2} \Delta E$.

$P_r(E, \bar{E}_r, X) \Delta E$, where $\bar{E}_r = \bar{E}_r(X)$ is given by B - 4.

4. Combined probability or yield of ions with energy $E_r(0) \pm \frac{1}{2} \Delta E_r$ from an incident beam of average energy $\bar{E}_i(0)$ permeating the total implanted region of the substrate.

$$Y(E_r)/\Delta E_r = c \int_0^\infty \rho(X) dX \int_0^\infty P_i(E, \bar{E}_i, X) \sigma(E) P_r(E, \bar{E}_r, X) dE.$$

D. Numerical Approximation (Computer Code BASS)

BASS is a FORTRAN code which calculates the value of $Y(E_r)/\Delta E_r$ for comparison with measured values of the same quantity, where ΔE is the channel width in a multichannel analyzer and E_r is proportional to channel number. The basic procedure is as follows:

- (a) The nuclear reaction parameters and substrate (target) properties are read.
- (b) Five values of the stopping powers in the expected energy region are read in for the incident and reaction ion followed by a least-squares fit of a third-order polynomial in each case in order to establish a continuous function of energy.

- (c) The spatial depth of the target (where the implanted ion density is appreciable) is divided into 100 segments X_j of width ΔX beginning at the surface of the target. At each of the 100 points below the surface, the energy of the incident ion is estimated by using approximation 4B where for each value of R in $S(R)$ the previous value $(R - \Delta X/\cos\alpha)$ is substituted, the ion energy having been already estimated there. In other words the $S(R)$ is found by iteration beginning at the surface where the energy is just E_i .
- (d) For each of the 100 values of incident ion energy E_i determined in (c), the corresponding value of E_r is determined by the formula of nonrelativistic kinematics. For each of these values of E'_r , the same procedure as in (c) is used to calculate the energy loss of the reaction ion as it leaves the reaction site and traverses to the target surface. Then $E_r = E'_r - \Delta E$ is computed.
- (e) For each of the 100 target depth positions X_j , the straggling and multiple scattering (B.1) values are computed for the incident ion traveling from the surface to X_j and the reaction ion leaving X_j and returning to the surface. For each of these values the beam spreading and detector resolution are added to the above straggling according to (B.3).
- (f) The differential reaction cross-section values for the incident-implanted ion reaction are read in along with the energies at which they have been measured (Rutherford cross sections — i.e., elastic scattering is calculated by the code when applicable). A polynomial least-squares fit is then made on this data in order to establish a continuous function $\sigma(E)$ in (C.4).
- (g) The mathematical parameters for either a split Gaussian or double Gaussian distribution for the implanted ions embedded in the substrate are then read in. For each of the 100 depths X_j the explicit value of $\rho(X_j)$ is computed.
- (h) The channel width ΔE_r is read in. For each channel energy of E_r desired, the double integral (C.4) is approximated as follows:

1. Each function of X is assumed to be constant over the range ΔX .
2. The lower limit of the energy-dependent integral is set to be the average energy of the incident ion after penetrating $100 \Delta X$ below the surface. The upper limit is taken as $E_i(0) + 2 \Omega_b$ in (B.2). The method of 3-point Gaussian quadrature is used to make the numerical evaluation. The appropriate integration step size was determined to be approximately 30 keV for total straggling values as low as 5 keV.
3. The lower limit for the spatial integral in (C.4) is taken as the target surface, 0, while the upper limit is $100 \Delta X$. Since discrete values of the integral are virtually determined, Simpson's rule was used to evaluate the spatial integral utilizing a $2 \Delta X$ integration sub-interval. The mathematical accuracy of the numerical methods are about 1%. Run time on the IBM 360-90 is approximately 1 s/channel or approximately 1 min for 60-point curve of the spectrum.

E. Input Format for BASS

Definition of terms given in appendix A or below. Units for the input and output terms are given in the code listing and below.

CARD	FORMAT	TERMS	UNITS
1	8F5.0	$E_i, M_i, Z_i, \alpha_i, Q, M_r, Z_r, \alpha_r, \alpha$	MeV, AMU, e, deg
2	8F5.0	M_s, Z_s, M_2, Z_2, N, T	$\text{g}\cdot\text{cm}^{-3}, \mu\text{m}$
3	8F5.0	ES1 ... ES5 energy of S1 values	MeV
4	8F5.0	S ₁₁ ... S ₁₅ , selected stopping power of incident ion	$\text{MeV}\cdot\mu\text{m}^{-1}$
5	8F5.0	W11 ... W15, weights of S1 values	if 1 leave blank
6-8	8F5.0	Same as 3-5 for reaction ion	
9	8F10.0	$\Omega_i(0), \Omega_d, \Delta\alpha_3$ (angle subtended by detector in reaction plane)	keV, deg
10	212	n,q number of σ data points and maximum polynomial fit to data (if blank, cards 11-13 omitted)	
11	14F5.0	ES1, ES2, ... ES _n - energy of σ	
12		S1, S2, ... S _n - σ values	
13		W1, W2, ... U _n - σ weights	
14-15	8E10.2 /E10.2	XB1, XB2, ... XB9 - parameters defining arbitrary density function in units of g/cm^3 (split Gaussian form)	
16	8F10.3	CALB, DCHAN - spectrum calibration and channel spacing in printout	keV/chan
17	F510	EXIT = -1 (stop), = 0 (start new case), - 1 (read new density cards 14-17)	

F. Listing of BASS

```

LEVEL 21.8 ( JUN 74 )                                CS/360 FORTRAN H

CCMPILER OPTIONS - NAME= EASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,EECDIC,NCLIST,DECK,LCAD,MAP,NOEDIT,IO,NCKREF

C***** BASS ***** BACK SCATTERING SPECTRA SIMULATION *****
C
ISN 0002      IMPLICIT REAL*(A-H,C-Z)
ISN 0003      DIMENSION S1(9), S3(9), W1(9), W3(9), ES1(9), ES3(9),
ISN 0004      2 FWR(9), VARNCE(9), ALFA(9), EETA(9), C(9)
ISN 0005      COMMON/51/EAV1(100), FAV2(100), THSUR ,DX, STPAG1(100),
ISN 0006      1 STPAG3(100), CELF(100)
ISN 0007      COMMON/52/E1,AM1,THETA1,013,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
ISN 0008      1 ZSUR,AMSUR
ISN 0009      COMMON/53/EC1,F1(9),CC3,D3(9)
ISN 0010      COMMON/54/ INDEX,NPCINT,NPCLY,NE3,IR,IW
ISN 0011      COMMON/55/ XF(9), FFC2(100), Y3(100)
ISN 0012      IR=5
ISN 0013      IW=6
ISN 0014      NPCWER = 3
ISN 0015      1000 WRITE(19,1)
ISN 0016      1 FORMAT(55H1 *** EASS *** BACKSCATTERING SPECTRA SIMULATION )
ISN 0017      WRITE(19,6)
ISN 0018      9 FORMAT(120H)1,2,3,4,SUR REFERS TO INCIDENT ICN, TARGET ATOM, REACT
ISN 0019      1 ICN ICN, RESIDUAL ICN, TARGET SUBSTRATE RESPECTIVLY )
ISN 0020      WRITE(19,2)
ISN 0021      2 FORMAT(55H0 E1 = INCIDENT ENERGY E3 = MAXIMUM FINAL ICN ENERGY )
ISN 0022      WRITE(19,3)
ISN 0023      3 FORMAT(55H0 V ,Z ,THETA = MASS CHARGE ANGLE FROM SURF. NORM. )
ISN 0024      WRITE(19,15)
ISN 0025      15 FORMAT(120H0 AMSLF,ZSUR= SLIPSTRATE MASS,CHARGE AM2,Z2 = TARGET MA
ISN 0026      1 SS,CHARGE RHC SLF,THSUR = SUBSTRATE DENSITY,THICKNESS )
ISN 0027      WRITE(19,4)
ISN 0028      4 FORMAT(55H0 S = DE/CX RFC TARGET DENSITY )
ISN 0029      WRITE(19,5)
ISN 0030      5 FORMAT(55H0 STPAG1,3 = FWHM ENERGY STRAGGLING IN E1, E3 )
ISN 0031      WRITE(19,6)
ISN 0032      6 FORMAT(55H0 CAV1,3 = AVERAGE ENERGY OF INCIDENT,FINAL ICN ENERGY )
ISN 0033      WRITE(19,7)
ISN 0034      7 FORMAT(55H0 UNITS = MEV,AML ,CEG.,MICRON, DENSITY=GRAMS/CC, MH/SR)
ISN 0035      WRITE(19,9)
ISN 0036      9 FORMAT(1HC)
ISN 0037      READ(IR,10) E1,AM1, Z1, THETA1, 013,AM3, Z3, THETA3
ISN 0038      10 FORMAT(8F5.0)
ISN 0039      WRITE(19,11) E1,AM1,Z1,THETA1,013,AM3,Z3,THETA3
ISN 0040      11 FORMAT(5HC E1=.F5.3 ,5H AM1=.F5.2 ,5H Z1=.F5.2 ,4H THETA1=. F5.1
ISN 0041      1,6H C13=.F5.2 ,5H AM3=.F5.2 ,5H Z3=.F5.2 ,4H THETA3=.F5.1)
ISN 0042      THETA1 = THETA1/57.3
ISN 0043      THETA3 = THETA3/57.3
ISN 0044      THETA=3.14159- THETA1-THETA3
ISN 0045      READ(IR,10) AMSLF, ZSUR, AM2, Z2, RHCSUR, THSUR
ISN 0046      WRITE(19,14)AMSUF, ZSUR, AM2, Z2, RHCSUB, THSUB
ISN 0047      14 FORMAT(8H0 AMSLF=.F5.0,6H ZSUR=.F5.0,5H AM2=.F5.0,4H Z2=.F5.0,
ISN 0048      19H RHCSUB=. F5.2, 4F THSUR=.F5.3)
ISN 0049      READ(IR,10)(ES1(K),K=1,3)
ISN 0050      READ(IR,10)(S1(K), K=1,5)
ISN 0051      READ(IR,10)(W1(K), K=1,3)
ISN 0052      READ(IR,10)(ES3(K),K=1,5)

```



```

ISN 0047      READ(IF,10)(S3(K), K=1,5)
ISN 0048      RFAC(IF,10)(W3(K), K=1,5)
ISN 0049      DO 100 I=1,5
ISN 0050      IF(W1(I).EQ.0) W1(I)=1.
ISN 0051      IF(W3(I).EQ.0) W3(I)=1.
ISN 0052      100 WRITE(IW,12)((ES1(K),K=1,5),(ES3(K),K=1,5))
ISN 0053      12 FORMAT(6H0 ES1=,E(2X,F5.2),6H ES3=,E(2X,F5.2))
ISN 0054      WRITE(IW,13)((S1(K),K=1,5),(S3(K),K=1,5))
ISN 0055      13 FORMAT(6H0 S1=,E(2X,F5.3),6H S3=,E(2X,F5.3))
ISN 0056      WRITE(IW,101)((W1(K),K=1,5),(W3(K),K=1,5))
ISN 0057      101 FORMAT(6H0 W1=,E(2X,F5.3),6H W3=,E(2X,F5.3))
ISN 0058      DX = THSLP/10.
ISN 0059      DELTAE = DEL(E1)
ISN 0060      WRITE(IW,125) DELTAE
ISN 0061      125 FORMAT(12H0 DE/DELTAE=, F10.6, 15H MEV PER DEGREE)
ISN 0062
ISN 0063      C
ISN 0064      C ENERGY LOSS FUNCTIONS
ISN 0065      125 CALL ORTHOG ( 5, FS1, S1, W1,ALFA,BETA,VARNCE,CC,C,ERC,ERR,NPOWER,
ISN 0066      1 NBFSTN,0, 0, 1, CC1,D1,0)
ISN 0067      WRITE(IW,16) VARNCE(2), D01,C1(1),D1(2),D1(3)
ISN 0068      16 FORMAT(5H0VARNCE=,F6.2,5H D1=,E(2X,F6.2))
ISN 0069      CALL ORTHOG ( 5, FS2, S3, W3,ALFA,BETA,VARNCE,CC,C,ERC,ERR,NPOWER,
ISN 0070      1 NBFSTN,C, 0, 1, CC3,D3,0)
ISN 0071      WRITE(IW,17) VARNCE(2), D03,C3(1),D3(2),D3(3)
ISN 0072      17 FORMAT(5H0VARNCE=,F6.2,5H D3=,E(2X,F6.2))
ISN 0073      DO 19 K=1,5
ISN 0074      FFS1(K)
ISN 0075      SX1 = CC1 + C1(1)*F + D1(2)*E**2 + D1(3)*E**3
ISN 0076      FFS3(K)
ISN 0077      SX3 = CC3 + C3(1)*F + D3(2)*E**2 + D3(3)*E**3
ISN 0078      19 WRITE(IW,21) SX1,SX3
ISN 0079      21 FORMAT(4H0S1 CAL=,F5.3,9H S3 CAL=,F5.3)
ISN 0080      WRITE(IW,18)
ISN 0081      18 FORMAT(120H1  )
ISN 0082      1 0THET1  EAV3  STRAG3  CTHET3  EAV1  STRAG1  )
ISN 0083
ISN 0084      C
ISN 0085      C AVERAGE ENERGIES PELCW SURFACE
ISN 0086      CALL EAV
ISN 0087
ISN 0088      C
ISN 0089      C MULTIPLE SCATTERING, STRAGGLING
ISN 0090      DO 201 I=1,100
ISN 0091      CTHET1=CSQRT(1.8  *2SUB/AM1*(EAV1(1)-EAV1(1))/EAV1(2+1/3))*2.36
ISN 0092      201 DELC(1) = CTHET1*DELC(EAV1(1/2))
ISN 0093      CALL STRAG
ISN 0094      DO 200 I=1,100
ISN 0095      X1 = CX*(I-1)
ISN 0096      R1 = X1/CCCS(1,FETA1)
ISN 0097      R3 = X1/CCCS(1,FETA3)
ISN 0098      CTHET1=CSQRT(1.8  *2SUB/AM1*(EAV1(1)-EAV1(1))/EAV1(2+1/3))*2.36
ISN 0099      EAV33 = E3(EAV1(1)) + 1.0-6
ISN 0100      CTHET3=CSQRT(1.8  *2SUB/AM3*(EAV33 - EAV3(1))/EAV3(2+1/3))*2.36
ISN 0101      200 WRITE(IW,23) X1,R1,R3,EAV1(1),STRAG1(1),DTHET1,
ISN 0102      1 EAV3(1),STRAG3(1),CTHET3
ISN 0103      20 FORMAT(10(4X,F6.2))
ISN 0104
ISN 0105      C
ISN 0106      C CROSS SECTION FUNCTION
ISN 0107      READ (IR,300)NFCINT,NPOLY
ISN 0108      300 FORMAT(2I2)
ISN 0109
ISN 0110      WRITE(IW,310) NFCINT , NPOLY
ISN 0111      310 FORMAT(5H1 NFCINT=,I2,7H NPOLY=,I2)
ISN 0112      IF(NPCINT.EQ.0) GO TO 400
ISN 0113      READ (IR,301) (S1(N),N=1,NPCINT)
ISN 0114      READ (IR,301) (S1(N),N=1,NPCINT)
ISN 0115      READ (IR,301) (W1(N),N=1,NPCINT)
ISN 0116      301 FORMAT(14F5.0)
ISN 0117      DO 305 I=1,9
ISN 0118      IF(W1(I).EQ.0) W1(I)=1.
ISN 0119      WRITE(IW,306)(FS1(N),N=1,NPCINT)
ISN 0120      WRITE(IW,306)( S1(N),N=1,NPCINT)
ISN 0121      WRITE(IW,306)( W1(N),N=1,NPCINT)
ISN 0122      306 FORMAT(11H0SIG. DATA ,10F9.3)
ISN 0123      IF(NPOINT.GT.0)CALL ORTHOG(NFCINT,ES1,S1,W1,ALFA,BETA,VARNCE,
ISN 0124      1 CC,C,ERC,BFA,NFCLY,NEESTN,0,0,1,D01,D1,0)
ISN 0125      WRITE(IW,308) (VARNCE(N),N=1,NFCLY)
ISN 0126      308 FORMAT(5H0 VARNCE=, F(2X,F5.3))
ISN 0127      WRITE(IW,307) CC1, (C1(N),N=1,NPOLY)
ISN 0128      307 FORMAT(4H0 D=, E(2X,F5.3))
ISN 0129      WRITE(IW,302)
ISN 0130      302 FORMAT(55H0 ENERGY SIGMA WSIG CALSIG )
ISN 0131      DO 303 N = 1,NPCINT
ISN 0132      CALSIG = SIGMA(ES1(N))
ISN 0133      303 WRITE(IW,304)ES1(N),S1(N), W1(N),CALSIG
ISN 0134      304 FORMAT( 5(2X,F5.2))
ISN 0135
ISN 0136      C
ISN 0137      C TARGET DENSITY
ISN 0138      401 CALL RECTMC
ISN 0139
ISN 0140      C
ISN 0141      C CONVOLUTION INTEGRALS
ISN 0142      CALL YIELD
ISN 0143      RFAC(IF,301) E*IT
ISN 0144      IF(FXIT) GOCC,10CC,401
ISN 0145      600 STOP
ISN 0146      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

COMPILER OPTIONS - NAME= EASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,ECCDIC,NCLIST,DECK,LOAD,MAP,NOEDIT,IO,NCXREF

```

ISN 0002      SUBROUTINE EAV
ISN 0003      IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004      COMMON/BI/EAV1(100),EAV3(100),THSUB,DX,STRAG1(100),
1 STRAG3(100),DELF(100)
ISN 0005      COMMON/B2/E1,AM1,THETA1,Q13,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
1 ZSUB,AMSLR
ISN 0006      COMMON/E3/CO1,(1(5),CO3,D3(9)
ISN 0007      EAV1(1)=E1
ISN 0008      EAV3(1)=E3(E1)
ISN 0009      DO 200 I=1,99
ISN 0010      E = EAV1(I)
ISN 0011      SX1 = CO1 + D1(1)*E + D1(2)*E**2 + D1(3)*E**3
ISN 0012      FAV1(I+1)= EAV1(I) - SX1 *DX/DCOS(THETA1)
ISN 0013      IF(EAV1(I+1).LT.1.E-6) FAV1(I+1)=1.E-6
ISN 0015      FAV3(I+1) = E3(EAV1(I+1))
ISN 0016      DO 100 K = 1,1
ISN 0017      E = FAV3(I+1)
ISN 0018      SX3 = CO3 + D3(1)*E + D3(2)*E**2 + D3(3)*E**3
ISN 0019      EAV3(I+1) = FAV3(I+1)-SX3 *DX/DCOS(THETA3)
ISN 0020      IF(EAV3(I+1).LT.1.E-6) EAV3(I+1)=1.E-6
ISN 0022      100 CONTINUE
ISN 0023      200 RETURN
ISN 0024      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

COMPILER OPTIONS - NAME= EASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,ECCDIC,NCLIST,DECK,LOAD,MAP,NOEDIT,IO,NCXREF

```

ISN 0002      SUBROUTINE STRAG
ISN 0003      IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004      COMMON/BI/EAV1(100),EAV3(100),THSUB,DX,STRAG1(100),
1 STRAG3(100),DELF(100)
ISN 0005      COMMON/B2/E1,AM1,THETA1,Q13,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
1 ZSUB,AMSLR
ISN 0006      COMMON/E4/ INDEX,NFCINT,NPCLY,NE3,IP,IM
100 CONTINUE
ISN 0007      C
ISN 0008      C
ISN 0009      C
ISN 0010      READ (IP,10) STRAG, STRAG1, DTHETA
100 FORMAT(RF10.0)
ISN 0011      WRITE (IM,5) STRAG, STRAG1, DTHETA
5 FORMAT(12H0 BEAM STRAG=F6.3,18H INSTRUMENT STRAG=F6.3,
1 12H APER ANGLE=F4.1)
ISN 0012      STRAG1(1) = STRAG
ISN 0013      STRAG3(1) = DSQRT(STRAG1**2+(DTHETA*DELF(1))**2)
ISN 0014      DO 1 IF=2,100
ISN 0015      T=DX*(I-1)
ISN 0016      T=T*1.E-4
ISN 0017      FOURPI = 12.566
ISN 0018      AVAGAD=F6.02023
ISN 0019      F4 = 2.07E-20
ISN 0020      S1 = FOURPI*21**2*2*SLF*F4
ISN 0021      S3 = FOURPI*23**2*2*SLF*F4
ISN 0022      S1=S1*AVAGAD*H*DELF*1/(DCOS(THETA1)*AMSUB)
ISN 0023      S3=S3*AVAGAD*H*DELF*1/(DCOS(THETA3)*AMSUB)
ISN 0024      STRAG1(1) = 2.36*DSQRT(S1+(STRAG/2.36)**2)
1 STRAG3(1) = 2.36*DSQRT(S3+(STRAG1/2.36)**2+(DELF(1)/2.36)**2)
1 DTHETA*DELF(EAV1(1)/2.36)**2)
ISN 0025      RETURN
ISN 0026      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

CCMPILER OPTIONS - NAME= EASSI,OPT=02,LINECNT=60,SIZE=3000K,
SOURCE,ECCDIC,NOLIST,DECK,LOAD,MAP,NCEDIT,IO,NC>REF
ISN 0302      SUBROUTINE CRTGCG (NPTS,X,Y,W,ALFA,BETA,VARNCE,CC,C,ERR,NFIT, ORTH 0
              > NACTLL,LASTFT,ICETE,ICDEF,DC,C,ISCL) ORTH 5
C PROGRAM AUTHOR G. W. WESTLEY ORTH 10
C COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV., ORTH 15
C CAK RIDGE, TENN. ORTH 20
ISN 0303      REAL*8 X(1),Y(1),W(1),ALFA(1),BETA(1),VARNCE(1),C(1),ERR(1),CO, ORTH 25
              > ERD,WDIAG,MINVAR,ACFM,DELSQ,RTHS,D(1),SOFI,DSCPL1,SIGSCI,STOVE, ORTH 30
              > DC,ASCL,ESCL,R(40),PCL1,PCL2,PCL3,FOLY(22),NGML(21) ORTH 35
              INTEGER*4 CCNVC ORTH 40
ISN 0304      COMMON/JSIAMS,FOL1(100),POL2(100),POL3(100),WDIAG,DSCPL1,ESCL,ASCL ORTH 45
ISN 0305      IF (LASTFT.LF.0) GO TO 10 ORTH 50
ISN 0306      I=LASTFT ORTH 55
ISN 0307      NFIT = I+1 ORTH 60
ISN 0308      GO TO 150 ORTH 65
ISN 0309      10 DO 20 I=1,NPTS ORTH 70
ISN 0310      POL1(I)=0.0 ORTH 75
ISN 0311      20 POL2(I)=1.0 ORTH 80
ISN 0312      NACTLL=0 ORTH 85
ISN 0313      WDIAG=C.C ORTH 90
ISN 0314      DO 30 I=1,NPTS ORTH 95
ISN 0315      30 WDIAG=WDIAG+W(I) ORTH 100
ISN 0316      BETA(I)=0.0 ORTH 105
ISN 0317      DELSQ=0.0 ORTH 110
ISN 0318      DO 40 I=1,NPTS ORTH 115
ISN 0319      40 DELSQ=DELSQ+W(I)*Y(I)**2 ORTH 120
ISN 0320      IF (ISCL.EC.0) GO TO 50 ORTH 125
ISN 0321      RTHS = X(I) ORTH 130
ISN 0322      NORM = RTHS ORTH 135
ISN 0323      DO 60 I=2,NPTS ORTH 140
ISN 0324      IF (NORM.GE.X(I)) GO TO 50 ORTH 145
ISN 0325      NORM = X(I) ORTH 150
ISN 0326      50 IF (RTHS.LF.X(I)) GO TO 60 ORTH 155
ISN 0327      RTHS = X(I) ORTH 160
ISN 0328      60 CONTINUE ORTH 165
ISN 0329      ASCL = 4.10/(NORM-RTHS) ORTH 170
ISN 0330      BSCL = -2.C0 - ASCL*RTHS ORTH 175
ISN 0331      DO 70 I=1,NPTS ORTH 180
ISN 0332      70 X(I) = X(I)*ASCL + BSCL ORTH 185
ISN 0333      80 CONTINUE ORTH 190
ISN 0334      I=0 ORTH 195
ISN 0335      90 RTHS=0.0 ORTH 200
ISN 0336      DO 100 K=1,NPTS ORTH 205
ISN 0337      100 RTHS=RTHS+W(K)*Y(K)*POL2(K) ORTH 210
ISN 0338      SOFI=RTHS/WDIAG ORTH 215
ISN 0339      DSCPL1=DELSQ-SOFI**2*WDIAG ORTH 220
ISN 0340      DSCPL1 = DABS(DSCPL1) ORTH 225
ISN 0341      IN=NPTS-I-1 ORTH 230
ISN 0342      SIGSOT=0.00 ORTH 235
ISN 0343      IF (IN.GT.0) SIGSCI=DSCPL1/CFLOAT(IN) ORTH 240
ISN 0344      STOVE = SIGSCI/WDIAG ORTH 245
ISN 0345      IF (I.EC.0) GO TO 110 ORTH 250
ISN 0346      C(I)=SOFI ORTH 255
ISN 0347      ERR(I)=STOVE ORTH 260
ISN 0348      VARNCE(I)=SIGSCI ORTH 265
ISN 0349      IF (I.EC.1) MINVAR=VARNCE(I) ORTH 270
ISN 0350      GO TO 120 ORTH 275

```

```

ISN 0059      110 CO=SOFI
ISN 0060      FRC=STEVE
ISN 0061      12) CONTINUE
ISN 0062      IF (I.EG.0) GO TO 130
ISN 0064      IF (VARNCE(I).GE.MINVAR) GO TO 130
ISN 0066      MINVAR=VARNCE(I)
ISN 0067      NACTUL=I
ISN 0068      13) CONTINUE
ISN 0069      140 IF (I.GE.NFIT) GO TO 220
ISN 0071      150 CO 160 K=1,NPTS
ISN 0072      160 POL2(K)=X(K)*FCL2(K)
ISN 0073      NCRM=0.00
ISN 0074      DO 170 K=1,NPTS
ISN 0075      170 NORM=NCRM+POL2(K)*W(K)*POL2(K)
ISN 0076      ALFA(I+1)=NCRM/NCIAG
ISN 0077      DO 180 K=1,NPTS
ISN 0078      180 POL3(K)=FCL2(K)-ALFA(I+1)*FCL2(K)-BETA(I+1)*POL1(K)
ISN 0079      NCRM=0.00
ISN 0080      DO 190 K=1,NPTS
ISN 0081      190 NCRM=NCRM+POL3(K)**2*W(K)
ISN 0082      I=I+1
ISN 0083      DO 200 K=1,NPTS
ISN 0084      200 POL1(K)=FCL2(K)
ISN 0085      POL2(K)=FCL3(K)
ISN 0086      BETA(I+1)=NCRM/NCIAG
ISN 0087      NCIAG=NCRM
ISN 0088      CELSO=CEGCLI
ISN 0089      GO TO 50
ISN 0090      22) CONTINUE
ISN 0091      IF (ICOFF.EG.0) RETURN
ISN 0093      A = NFIT
ISN 0094      IF (IDETR.NE.0) A = NACTUL
ISN 0096      CO 230 I=1,N
ISN 0097      23) C(I) = 0.00
ISN 0098      POLY(1) = 0.00
ISN 0099      POLY(2) = 0.00
ISN 0100      NCML(1) = 1.00
ISN 0101      DO = CO
ISN 0102      DO 260 I=1,N
ISN 0103      DO 250 J=1,I
ISN 0104      NCRM = FCLY(J+1)*BETA(I)
ISN 0105      FCLY(J+1) = NCML(J)
ISN 0106      NCML(J) = FCLY(J) - ALFA(I)*NCML(J) - NCRM
ISN 0107      IF (J.GT.1) GO TO 240
ISN 0108      DO = CC + C(I)*NCML(J)
ISN 0109      GO TO 250
ISN 0110      240 KA = J-1
ISN 0111      C(KA) = C(KA) + C(I)*NCML(J)
ISN 0112      250 CONTINUE
ISN 0113      C(I) = C(I)
ISN 0114      NCML(I+1) = 1.00
ISN 0115      POLY(I+2) = 0.00
ISN 0116      250 CONTINUE
ISN 0117      IF (ISCL.EG.0) RETURN
ISN 0118      NCRM = 1.00
ISN 0120      POLY(1) = 1.00
ISN 0121      R(1) = BSCL
ISN 0122      RTHS = CC + C(1)*R(1)
ISN 0123

```

ORTH 280
 ORTH 285
 ORTH 290
 ORTH 295
 ORTH 300
 ORTH 305
 ORTH 310
 ORTH 315
 ORTH 340
 ORTH 345
 ORTH 350
 ORTH 355
 ORTH 360
 ORTH 365
 ORTH 370
 ORTH 375
 ORTH 380
 ORTH 385
 ORTH 390
 ORTH 395
 ORTH 400
 ORTH 405
 ORTH 410
 ORTH 415
 ORTH 420
 ORTH 425
 ORTH 430
 ORTH 435
 ORTH 440
 ORTH 445
 ORTH 450
 ORTH 455
 ORTH 460
 ORTH 465
 ORTH 470
 ORTH 475
 ORTH 480
 ORTH 485
 ORTH 490
 ORTH 495
 ORTH 500
 ORTH 505
 ORTH 510
 ORTH 515
 ORTH 520
 ORTH 525
 ORTH 530
 ORTH 535
 ORTH 540
 ORTH 545
 ORTH 550
 ORTH 555
 ORTH 560
 ORTH 565
 ORTH 570
 ORTH 575
 ORTH 580
 ORTH 585
 ORTH 590

```

ISN 0124      IF (N.EG.1) GO TO 280
ISN 0126      CC 270 I=2,N
ISN 0127      POLY(I) = 1.00
ISN 0128      R(I) = BSCL*R(I-1)
ISN 0129      270 RTHS = RTHS + C(I)*R(I)
ISN 0130      280 CONTINUE
ISN 0131      DO 320 J=1,N
ISN 0132      NCRM = NCRM + ASCL
ISN 0133      NCML(J) = C(J)*NCRM
ISN 0134      K = 1
ISN 0135      I = J+1
ISN 0136      290 IF (I.GT.N) GO TO 320
ISN 0138      POLY(K) = ASCL*FCLY(K)
ISN 0139      IF (K.EG.1) GO TO 300
ISN 0141      POLY(K) = FCLY(K) + FCLY(K-1)
ISN 0142      GO TO 310
ISN 0143      300 POLY(K) = FCLY(K) + NCRM
ISN 0144      310 NCML(J) = NCML(J) + C(I)*POLY(K)*R(K)
ISN 0145      K = K+1
ISN 0146      I = I+1
ISN 0147      GO TO 290
ISN 0148      320 CONTINUE
ISN 0149      DO = RTHS
ISN 0150      DO 330 I=1,N
ISN 0151      330 D(I) = NCML(I)
ISN 0152      RETURN
ISN 0153      END

```

ORTH 595
 ORTH 600
 ORTH 605
 ORTH 610
 ORTH 615
 ORTH 620
 ORTH 625
 ORTH 630
 ORTH 635
 ORTH 640
 ORTH 645
 ORTH 650
 ORTH 655
 ORTH 660
 ORTH 665
 ORTH 670
 ORTH 675
 ORTH 680
 ORTH 685
 ORTH 690
 ORTH 695
 ORTH 700
 ORTH 705
 ORTH 710
 ORTH 715
 ORTH 720
 ORTH 725

LEVEL 21.8 (JUN. 74)

CS/36J FORTRAN H

```

      CCMPILER OPTIONS - NAME= EASS1,OPT=07,LINECNT=60,SIZE=0030K,
                        SOURCE,EECCIC,ACLIST,DECK,LOAD,MAP,NCEDIT,IO,ACXREF
      ISN 0002      SUBROUTINE RHC2HC
      ISN 0003      IMPLICIT REAL*8 (A-H,O-Z)
      ISN 0004      COMMON/81/EAV1(100), EAV3(100), THSUB ,DX, STRAG1(100),
      ISN 0005      1 STRAG3(100),DELE(100)
      ISN 0006      COMMON/84/ INDEX,NCINT,NCGLY,NEW,IR,IX
      ISN 0007      COMMON/85/ XF(5), RHC2(100), Y3(100)
      ISN 0008      READ(IR,30)(XE(I),I=1,9)
      ISN 0009      30 FORMAT(5E10.2,/,E10.2)
      ISN 0010      WRITE(IX,21)(YE(I),I=1,9)
      ISN 0011      21 FORMAT(5H1 I=,E5.2,4H 2=,E9.2,4H 3=,E9.2,4H 4=,E9.2,4H 5=,
      ISN 0012      1E9.2,4H 6=,E9.2,4H 7=,E9.2,4H 8=,E9.2,4H 9=,E9.2)
      ISN 0013      WRITE(IX,35)
      ISN 0014      35 FORMAT(55H0 RHC2 INTEG LIMIT=10-6 G/CM-3 THIS IS SFT IN YIELD )
      ISN 0015      20 FORMAT(55H0 > RHC2CN RHC2 G/CM-3 AREA MG/CM-2 )
      C
      C      INITIAL TARGET DENSITY FUNCTION IS DEFINED HERE
      C
      C      XR1 = BEGIN STEP FUNCTION(MICRONS)
      C      XR2 END STEP FUNCTION(MICRONS)
      C      XR3 = STEP HEIGHT(G/CC)
      C
      C      XR4 = GAUSS1 CENTER(MICRONS)
      C      XR5 = GAUSS1 AREA(.1MG/CM2)
      C      XR6 = GAUSS1 WIDTH(50)(MICRONS)
      C      XR7 = GAUSS2 CENTER
      C      XR8 = GAUSS2 AREA
      C      XR9 = GAUSS2 WIDTH(50)
      C
      ISN 0015      XR(6) = 1.0-10 + XF(6)
      ISN 0016      XR(9) = 1.0-10 + XF(9)
      ISN 0017      RTWOP1 = 2.306
      ISN 0018      AREA = 0.
      ISN 0019      DO 10 I=1,100
      ISN 0020      X = DX*(I-1)
      ISN 0021      IF(X.LT.XE(1)) RHC2(I) = 0.
      ISN 0022      IF(X.GE.XF(1)) RHC2(I) = XE(1)
      ISN 0023      IF(X.LT.XF(2)) RHC2(I) = 0.
      ISN 0024      IF(X.GE.XF(2)) RHC2(I) = XE(2)
      ISN 0025      P1 = ((X-XE(4))/(1.414*XR(6)))**2
      ISN 0026      P2 = ((X-XE(7))/(1.414*XR(9)))**2
      ISN 0027      IF(P1.LT.100.) P1=100.
      ISN 0028      IF(P2.LT.100.) P2=100.
      ISN 0029      GAUS1 = (XE(5)/(XE(6)*RTWOP1))*EXP(-P1)
      ISN 0030      GAUS2 = (XE(8)/(XE(9)*RTWOP1))*EXP(-P2)
      ISN 0031      IF(X.LT.XE(4)) RHC2(I) = RHC2(I) + GAUS1
      ISN 0032      IF(X.GE.XF(4)) RHC2(I) = RHC2(I) + XR(5)/(XE(6)*RTWOP1)
      ISN 0033      IF(X.LT.XE(7)) RHC2(I) = RHC2(I) - XR(5)/(XE(6)*RTWOP1)
      ISN 0034      IF(X.GE.XF(7)) RHC2(I) = RHC2(I) - XR(5)/(XE(6)*RTWOP1) + GAUS2
      ISN 0035      AREA = AREA+RHC2(I)*DX*.1
      ISN 0036      1) WRITE(IX,21) X, RHC2(I), AREA
      ISN 0037      2) FORMAT (F10.2,/,F10.3)
      ISN 0038      RETURN
      ISN 0039      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

CCMPILER OPTIIONS - NAME= FASS1,OPT=02,LINECNT=60,SIZE=0000K,
                    SOURCE,PRECIC,NOLIST,DECK,LOAD,MAP,NOEDIT,LD,NCXFEF
ISN 0002      SUBROUTINE YIELD
ISN 0003      IMPLICIT REAL*8 (A-H,C-Z)
ISN 0004      EXTERNAL F3KERN, F1KERN
ISN 0005      COMMON/E1/EAV1(100), EAV3(100), THSUP ,DX, STRAG1(100),
ISN 0006      1 STRAG3(100),DELE(100)
ISN 0006      COMMON/B2/E1,AM1,THETA1,013,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
ISN 0007      1 ZSUR,AMSLR
ISN 0007      COMMON/24/ INDEX,NPCINT,NPCLY,NE3,IP,1W
ISN 0108      COMMON/RS/ XE(C), F+C2(100) , Y3(100)
C
ISN 0009      RFAC(IP,34) (ALB, DCHAN
ISN 0010      FACT = 1000/CALB
ISN 0011      34 FCFMAT(EF10,3)
ISN 0012      SHIFT = (STRAG1(2) + STRAG3(2))*2.*DCHAN/DABS(DCHAN)
ISN 0013      YNCRM = 3.76D+(2/AM2
ISN 0014      EIMIN=EAV1(100)
ISN 0015      EM = E1 + 2.*STRAG1(1)
ISN 0016      NST=(E1-EIMIN)/.1D + 1D
ISN 0017      WRITE(1W,35) CALB,DCHAN
ISN 0018      35 FCFMAT(7H1 CALB=,F4.3,9H KEV/CHAN,7H DCHAN=,F5.2)
ISN 0019      WRITE(1W,32)
ISN 0020      32 FCFMAT(53HC      E3      CHANNEL      CTS/CHAN/MICR/MSR      SUM )
ISN 0021      SYIELD = 0.
ISN 0022      DO 101 NE3 = 1,100
ISN 0023      EAV3(NE3) = EAV3(1)-(NE3-1)*CCHAN/FACT + SHIFT
ISN 0024      CHAN = EAV3(NE3)*FACT
ISN 0025      IF(EAV3(NE3) .LT. 1.D-2) NE3=100
ISN 0027      YIELD3= 0.
ISN 0028      DO 100 INDEX = 1, 100
ISN 0029      Y3(INDEX) = 0.
ISN 0030      IF(RHC2(INDEX).LT.1.D-06)GC TC 103
ISN 0032      CALL INTEGR(EIMIN,EM,NST,CCNV,E1KERN)
ISN 0033      PROD = RHC2(INDEX)*CCNV*YNCRM*DX/DCOS(THETA1)
ISN 0034      Y3(INDEX)=PROD/FACT
ISN 0035      100 CONTINUE
C
C      INTEGRATION VIA SIMPSON RULE = YIELD3
ISN 0036      S1 = 0
ISN 0037      S2 = 0
ISN 0038      DO 102 J=3,57,2
ISN 0039      102 S1 = S1+Y3(J)
ISN 0040      DO 103 J=2,56,2
ISN 0041      103 S2 = S2+Y3(J)
ISN 0042      YIELD3 = 0.333*(Y3(1)+Y3(59))+2.*S1+4.*S2)
ISN 0043      SYIELD = SYIELD+YIELD3*DARS(DCHAN)
C
ISN 0044      TEST = SYIELD/YIELD3
ISN 0045      IF(TEST.GT.8000) NE3=100
ISN 0047      101 WRITE(1W,33) EAV3(NE3),CHAN,YIELD3,SYIELD
ISN 0048      33 FCFMAT(F10.3,5X,F10.3,5X,2(F10.3,5X))
ISN 0049      RETURN
ISN 0050      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

CCMPILER OPTIIONS - NAME= FASS1,OPT=02,LINECNT=60,SIZE=0000K,
                    SOURCE,PRECIC,NOLIST,DECK,LOAD,MAP,NOEDIT,LD,NCXFEF
ISN 0002      DOUBLE PRECISION FUNCTION DEL(E)
ISN 0003      IMPLICIT REAL*8 (A-H,C-Z)
ISN 0004      COMMON/E2/E1,AM1,THETA1,013,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
ISN 0005      1 ZSUR,AMSLR
ISN 0006      THETA = THETA-1./57.3
ISN 0006      E1 = E3(E)
ISN 0007      THETA = THETA+1./57.3
ISN 0008      EF = F3(E)
ISN 0009      DEL = E1-EF
ISN 0010      RETURN
ISN 0011      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

COMPILER OPTIONS - NAME= FASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,ECCIC,NCLIST,CECK,LOAD,MAP,NCECIT,10,NCXREF
ISN 0002 DOUBLE PRECISION FUNCTION E3(E)
ISN 0003 IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004 COMMON/92/E1,AM1,THETA1,Q13,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
1 ZSUB,ANSUE
ISN 0005 IF(E.LT.1.0- $\epsilon$ ) E=1.0- $\epsilon$ 
ISN 0006 AM4 = AM1+AM2 - AM3
ISN 0007 V = AM1*AM3*E
ISN 0008 V = V**5*ECCS(THETA)/(AM3+AM4)
ISN 0009 W = AM4*Q13 + E*(AM4-AM1)
ISN 0010 W = W/(AM3+AM4)
ISN 0011 E3 = V + (V**2 + W)**.5
ISN 0012 E3=E3**2
ISN 0013 RETURN
ISN 0014
ISN 0015 END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

COMPILER OPTIONS - NAME= FASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,ECCIC,NCLIST,CECK,LOAD,MAP,NCECIT,10,NCXREF
ISN 0002 DOUBLE PRECISION FUNCTION SIGMA(E)
ISN 0003 IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004 COMMON/92/E1,AM1,THETA1,Q13,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
1 ZSUB,ANSUE
ISN 0005 COMMON/E3/DC1,C1(7),CC3,C3(9)
ISN 0006 COMMON/E4/ INDEX,NPCINT,NPCLY,NE3,IR,IW
C
C NPCINT < 3 FOR ARBITRARY FUNCTION
C NPCINT = 0 FOR FLTHREFFORD SCATTERING
C NPCINT > 0 FOR LEAST SQUARES FIT FUNCTION
C
ISN 0007 IF(NPCINT)1,2,3
ISN 0008 1 SIGMA = 1.0
ISN 0009 GO TO 10
ISN 0010 2 R = 1.44*71*Z2/E
ISN 0011 SIGMAH = 1./DSIN(THETA/2)**4 - 2.*(AM1/AM2)**2
ISN 0012 SIGMA = (3/4)**2*IC.*SIGLAH
ISN 0013 GO TO 10
ISN 0014 3 SIGMA = DC1
ISN 0015 DO 4 I=1,NPCLY
ISN 0016 4 SIGMA = SIGMA + C1(I)*F**I
ISN 0017 10 IF(SIGMA .LT. (.)) SIGMA=0.
ISN 0018 RETURN
ISN 0019
ISN 0020 END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

COMPILER OPTIONS - NAME= FASS1,CPT=02,LINECNT=60,SIZE=0000K,
SOURCE,ECCIC,NCLIST,CECK,LOAD,MAP,NCECIT,10,NCXREF
ISN 0002 DOUBLE PRECISION FUNCTION EIKERN(E)
ISN 0003 IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004 COMMON/R1/FAV1(100),EAV3(100),THSUB,DX,STRAG1(100),
1 STRAG3(100),CELE(100)
ISN 0005 COMMON/32/E1,AM1,THETA1,Q13,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
1 ZSUB,ANSUE
ISN 0006 COMMON/P4/ INDEX,NPCINT,NPCLY,NE3,IR,IW
ISN 0007 EIKERN = FPRCP(E, EAV1(INDEX), STRAG1(INDEX))
ISN 0008 EIKERN = EIKERN * SIGMA(E)
ISN 0009 EIKERN = EIKERN * F2KERN(E)
ISN 0010 RETURN
ISN 0011 END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

      COMPILER OPTIONS - NAME= FASS1,CPT=02,LINECNT=60,SIZE=0000K,
                        SOURCE,ECCIC,NOLIST,CECK,LOAD,MAP,NCEEDIT,ID,NCREF
      ISN 0002      DOUBLE PRECISION FUNCTION E3KERN(E)
      ISN 0003      IMPLICIT REAL*8 (A-F,C-Z)
      ISN 0004      COMMON/81/EAV1(100), EAV3(100), THSUB ,DX, STRAG1(100),
      ISN 0005      1 STRAG2(100),DELE(100)
      ISN 0006      COMMON/82/E1,AM1,THETA1,013,AM3,THETA3,AM2,Z1,Z2,Z3,THETA,RHOSUB,
      ISN 0007      1 ZSUB,AMSLF
      ISN 0008      COMMON/83/CC1,C1(9),C(3,03(9)
      ISN 0009      COMMON/84/ INDEX,NFCINT,NPCLY,NE3,IR,1W
      ISN 0010      EAV33 = E3(E)
      ISN 0011      DO 100 K = 1,INDEX
      ISN 0012      F = EAV33
      ISN 0013      SX3 = CC3 + C3(1)*F + C3(2)*F**2 + C3(3)*F**3
      ISN 0014      100 EAV33 = EAV33 - SX3*CX/PCOS(THETA3)
      ISN 0015      IF(EAV33.LT.1.C-06) EAV33=1.C-06
      ISN 0016      F3KERN = EPRCEX(EAV3(NE3 ), EAV33, STRAG3(INDEX))
      ISN 0017      RETURN
      ISN 0018      END

```

LEVEL 21.8 (JUN 74)

CS/360 FORTRAN H

```

      COMPILER OPTIONS - NAME= FASS1,CPT=02,LINECNT=60,SIZE=0000K,
                        SOURCE,ECCIC,NOLIST,CECK,LOAD,MAP,NCEEDIT,ID,NCREF
      ISN 0002      DOUBLE PRECISION FUNCTION EPRCEX(E,EAV,STRAG)
      ISN 0003      IMPLICIT REAL*8 (A-F,C-Z)
      ISN 0004      SIGMA = STRAG/2.36
      ISN 0005      EX=( (F-EAV)/(1.414*SIGMA) )**2
      ISN 0006      IF(EX.GT.20.) EX = 20.
      ISN 0007      EPRCEX = 0EXP( -EX )/(2.507*SIGMA)
      ISN 0008      RETURN
      ISN 0009      END

```


THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

INTERNAL DISTRIBUTION

1-2. Central Research Library	31. F. K. McGowan
3. Document Reference Section	32. C. J. McHargue
4-5. Laboratory Records Department	33. R. E. Pawel
6. Laboratory Records Department, RC	34. G. F. Peterson
7. ORNL Patent Section	35. H. E. Reesor
8. J. Bentley	36. T. C. Reiley
9. P. T. Carlson	37. J. O. Stiegler
10. R. W. Carpenter	38. T. N. Tiegs
11. L. C. Emerson	39. F. W. Wiffen
12. M. L. Grossbeck	40. N. J. Zaluzec
13-15. M. R. Hill	41. R. W. Balluffi (consultant)
16. E. H. Lee	42. W. R. Hibbard, Jr. (consultant)
17-26. M. B. Lewis	43. R. J. Jaffe (consultant)
27. J. S. Lin	44. M. J. Mayfield (consultant)
28. J. E. Mack	45. John Moteff (consultant)
29. L. K. Mansur	46. J. T. Stringer (consultant)
30. D. L. Mason	

EXTERNAL DISTRIBUTION

47. J. L. Brimhall, Pacific Northwest Laboratories, P. O. Box 999, Richland, WA 99352
48. W. J. Choyke, University of Pittsburgh, Westinghouse Research Laboratory, 1310 Beulah Road, Pittsburgh, PA 15235
49. M. M. Cohen, Office of Fusion Energy, U. S. Department of Energy, Washington, DC 20545
50. D. F. Cowgill, Sandia Laboratories, Livermore, CA 94551
51. L. C. Ianniello, Division of Materials Sciences, Office of Basic Energy Sciences, U. S. Department of Energy, Washington, DC 20545
52. G. L. Kulcinski, University of Wisconsin, 1500 Johnson Drive, Madison, WI 53706
53. S. T. Picraux, Sandia Laboratories, Albuquerque, NM 87115
54. F. A. Smidt, Engineering Materials Division, Naval Research Laboratory, Code 6390, Washington, DC 20375
55. John Spitznagel, Westinghouse Research Laboratory, 1310 Beulah Road, Pittsburgh, PA 15235
56. A. Taylor, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439
57. F. L. Vook, Sandia Laboratories, Albuquerque, NM 87115
58. H. Wiedersich, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439
59. Peter Wilkes, University of Wisconsin, 1500 Johnson Drive, Madison, WI 53706
60. S. M. Wolf, Division of Materials Sciences, Office of Basic Energy Sciences, U. S. Department of Energy, Washington, DC 20545

- 61. Assistant Manager, Office of Energy Research and Development,
DOE-ORO
- 62-88. Technical Information Center, Oak Ridge, TN 37830