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The Program RADELI for Evaluation of the
Moments over the Range- and Deposited Energy-
Distributions for Light Ion Bombardment
of Solids.

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ABSTRACT

A Computer program RADELI is described to calculate the moments of the range and deposited energy distributions for light ions in amorphous solids. The scheme of the classical work by Schiøtt and by Sigmund and Weissmann is followed, but more accurate approximations are used. The physical problem is described and the formulae necessary for the evaluation are presented. A detailed description of all subprograms contained in RADELI is given. Methods to construct a distribution from its moments are available but are not discussed in this note.

Zusammenfassung

Ein Computer-Programm, RADELI, zur Berechnung der Momente der Verteilungen sowohl der Reichweite als auch der deponierten Energie für leichte Ionen in amorphen Substanzen wird beschrieben. Die analytischen Rechnungen folgen dem Schema der klassischen Arbeiten von Schiøtt sowie von Sigmund und Weissmann. Es werden jedoch bessere Näherungen verwendet. Das physikalische Problem und die zu seiner Lösung notwendigen Gleichungen werden diskutiert. Der Bericht enthält ferner eine detaillierte Beschreibung aller in RADELI enthaltenen Unterprogramme. Die Methoden zur Konstruktion einer Verteilung aus ihren Momenten werden in dieser Arbeit nicht diskutiert.

1. INTRODUCTION.

The need for theoretically determined range and energy distributions for light ions in solids based on few, simple and well established assumptions has been steadily increasing during the latter years. Especially within disciplines like plasma wall interaction in fusion reactors these functions may be valuable. Classical works in the field are by Schiøtt /1/ and by Sigmund and Weissmann /2/.

In this note the scheme of these authors is followed but new and more accurate approximations are used. It should be stressed that the program presented here is based on analytical calculations. Simulation programs, such as MARLOWE /3/, are more flexible and at many points more physically relevant but are on the other hand limited in accuracy by statistics and the interpretation of the results is made difficult due to complexities in the assumptions.

In the following the physical problem is described and the formulae necessary for the evaluation are presented. The note ends up with a detailed discription of all subprograms contained in the RADELI sample program.

The program is designed only to calculate the moments over the distributions. Several methods to construct a distribution from its moments are available /4/, /5/, /6/, but as the problem of a suitable choice of construction method is not fully understood and more or less a question of intuition, it has been decided here only to present the objective information contained in the moments.

More details concerning the mathematical approaches used and comparisons with the results of ref. 1, 2, and 8 will be published later. A comparison with moments obtained with the simulation program MARLOWE, and applications of the RADELI results may be found in ref. 18, 19, and 20.

2. DESCRIPTION OF THE PROBLEM.

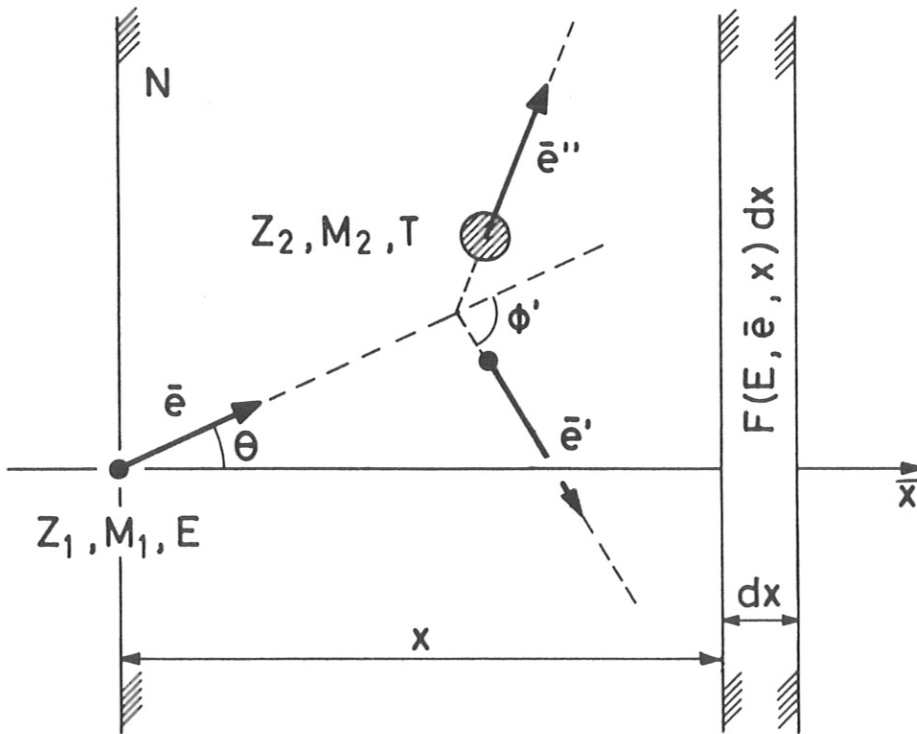


Fig. 1.

Schematic picture of the creation of a recoil atom in an elastic collision, the basic process leading to the deposition of magnitude $F(x)dx$ in a slice of material of thickness dx at depth x . See the text for the notations.

Consider a monoatomic, isotropic, homogenous, and infinite medium, consisting of resting atoms with mass M_2 and atomic number Z_2 , and with the density N . Let \bar{x} be an arbitrary axis and let an ion of mass M_1 with atomic number Z_1 start in $x=0$ in the direction \bar{e} with energy E . (consult fig. 1.)

We want to calculate: 1) the probability that the ion gets stopped in the slice (x, dx) , that is /7/ the ion range depth distribution (IR), 2) the energy deposited in atomic motion by the ion and all recoils in (x, dx) , when transport of energy no longer takes place over finite distances, that is /4/ the deposited nuclear energy distribution (DNE), 3) the energy deposited in electronic excitations in (x, dx) assuming these to be stable, that is /8/ the deposited electronic energy distribution (DEE), which is the complementary quantity to (DNE), and 4) the sum of 2) and 3), that is the deposited total energy distribution (DTE).

T r a n s p o r t e q u a t i o n .

Let the desired quantity be $F(E, \bar{e}, x) dx$. The linearized Boltzmann transport equation describing F is (refs. /4/, /9/)

$$-\cos\theta \frac{\partial F}{\partial x} - NS_e(E) \frac{\partial F}{\partial E} = N \int d\sigma \{ F(E, \bar{e}, x) - F(E-T, \bar{e}', x) - G(T, \bar{e}'', x) \} \quad (1)$$

where $\cos\theta = \cos(\bar{e}, \bar{x})$, $d\sigma = d\sigma(E, T)$ is the elastic scattering cross section for a binary collision in which an energy T is transferred from the ion with direction \bar{e} to a previously resting target atom now moving in the direction \bar{e}'' as a recoil. The new direction for the ion is \bar{e}' . It is assumed that the elastic and the inelastic energy losses are separable, the latter being summarized in the

electronic stopping power $NS_e(E)$. $G(E, \bar{e}, x)$ is a function describing the corresponding deposition by recoils only, and may be determined by substituting $F \rightarrow G$ in the above; the so called equal mass case. Implicit assumptions concerning the derivation of eq.(1) may be found in ref. /4/, and /9/.

L i g h t i o n c a s e .

The special cases of interest here are ion-target combinations for which $\mu = M_2/M_1 \gg 1$. As the maximum energy transfer

$$T_m = \gamma E = 4\mu(1+\mu)^{-2}E \quad (2)$$

is then much less than E , an expansion in T of the second term in the bracket of (1) is adequate, and to the first order we get

$$F(E-T, \bar{e}; x) = F(E, \bar{e}; x) - T \frac{\partial F}{\partial E} \quad (3)$$

Moreover the range of recoils is much shorter than the range of the ions which means that deposition by recoils may be regarded as strongly localized to the collision region, or that

$$G(T, \bar{e}''; x) \approx G(T) \delta(x) \quad (4)$$

where $\delta(x)$ is the Dirac delta function. For the (IR) case the recoils do not contribute and G should be set to zero.

Defining the moments over the distribution F as

$$F^n(E, \bar{e}) = \int_{-\infty}^{\infty} x^n F(E, \bar{e}, x) dx \quad (5)$$

and expanding the angular dependence in Legendre polynomials P_ℓ

$$F^n(E, \bar{e}) = \sum_{\ell=0}^{\infty} F_\ell^n(E) P_\ell(\cos\theta) \quad (6)$$

eq. (1) with (3) and (4) reduces to an equation for the coefficients F_ℓ^n

$$\frac{n}{2\ell+1} \{ \ell F_{\ell-1}^{n-1}(E) + (\ell+1) F_{\ell+1}^{n-1}(E) \} =$$

$$\{ NS_e(E) + I_1(\ell, E) \} \frac{d}{dE} F_{\ell}^n(E) + I_2(\ell, E) F_{\ell}^n(E)$$

$$- N \int d\sigma(E, T) G(T) \delta_{\ell 0} \delta_{n 0} \quad (7)$$

where

$$I_1(\ell, E) = N \int d\sigma(E, T) T P_{\ell}(\cos\phi') \quad (8)$$

$$I_2(\ell, E) = N \int d\sigma(E, T) (1 - P_{\ell}(\cos\phi')) \quad (9)$$

ϕ' being the scattering angle given by

$$\cos\phi' = (1-T/E)^{\frac{1}{2}} + \frac{1}{2}(1-\mu) T/E (1-T/E)^{-\frac{1}{2}} \quad (10)$$

Scattering integrals.

Equation (10) may more conveniently be written

$$\cos\phi' = (1-\gamma T/T_m)^{\frac{1}{2}} + \frac{1}{2}(1-\mu) \gamma T/T_m (1-\gamma T/T_m)^{-\frac{1}{2}} \quad (11)$$

where $T/T_m \in [0, 1]$, and remembering our interest in small values of $1/\mu$, we write to the first order in this quantity

$$\cos\phi' = 1 - 2 T/T_m + 4/\mu (T/T_m - T^2/T_m^2) \quad (12)$$

and

$$P_{\ell}(\cos\phi') \equiv \sum_{k=0}^{\ell} a_{\ell k} (\cos\phi')^k = \sum_{k=0}^{2\ell} c_{\ell k} (T/T_m)^k \quad (13)$$

The scattering integrals I_1 and I_2 then reduces to the simple forms

$$I_1(\ell, E) = T_m \sum_{k=0}^{2\ell} c_{\ell k} N \int d\sigma(E, T) (T/T_m)^{k+1} \quad (14)$$

$$I_2(\ell, E) = -\sum_{k=0}^{2\ell-1} c_{\ell, k+1} N \int d\sigma(E, T) (T/T_m)^{k+1} \quad (15)$$

Scattering cross section.

For the elastic scattering cross section $d\sigma$, we use the Lindhard expression /10/, which makes it convenient to transform all quantities into reduced units:

$$N d\sigma = \frac{\rho_0}{\gamma} \frac{dt}{2t^{3/2}} f(t^{1/2}) \quad (16)$$

where

$$t = T/T_m \epsilon^2 \equiv T/T_m (E\epsilon_0)^2 \quad (17)$$

$$\epsilon_0 = \mu((1+\mu)Z_1Z_2e^2)^{-1} a \quad (18)$$

$$\rho_0 = N\pi a^2 \gamma \quad (19)$$

with

$$/10/ \quad a = a_L \equiv 0.8853 a_0 (Z_1^{2/3} + Z_2^{2/3})^{-1/2} \quad (20L)$$

$$\text{or } /17/ \quad a = a_F \equiv 0.8853 a_0 (Z_1^{1/2} + Z_2^{1/2})^{-2/3} \quad (20F)$$

a_0 being the classical Bohr radius and $-e$ the electron charge.

For the function $f(t^{1/2})$ we use the Winterbon-approximation /11/

$$f(t^{1/2}) = \lambda t^{1/2-m} (1+(2\lambda t^{1-m})^q)^{-1/q} \quad (21)$$

which reduces the scattering integrals to

$$I_1(l, E) = \frac{\rho_0}{\epsilon_0} \epsilon^{1-2m} \lambda/2 \sum c_{lk} S(k, \epsilon) \equiv \frac{\rho_0}{\epsilon_0} i_1(l, \epsilon) \epsilon^{1-2m} \quad (22)$$

$$I_2(l, E) = - \frac{\rho_0}{\gamma} \epsilon^{-2m} \lambda/2 \sum c_{l, k+1} S(k, \epsilon) \equiv \frac{\rho_0}{\gamma} i_2(l, \epsilon) \epsilon^{-2m} \quad (23)$$

where

$$S(k, \epsilon) = \int_0^1 y^{k-m} (1+(2\lambda \epsilon^{2-2m} y^{1-m})^q)^{-1/q} dy \quad (24)$$

For sufficiently small energies we find

$$S(k, \epsilon) = S(k) = (1+k-m)^{-1} \quad (24a)$$

Electronic energy loss.

In equation (1) it is assumed that the net result of the interaction projectile-electrons, apart from nuclear charge screening, is only an energy loss per unit path length $\left. \frac{dE}{dx} \right|_e$. In reduced units and using Lindhards expression /7/,

$$\frac{\epsilon_0}{\rho_0} \left. \frac{dE}{dx} \right|_e = \frac{\epsilon_0}{\rho_0} NS_e(E) = \frac{d\epsilon}{d\rho} = k\sqrt{\epsilon} = s_e(\epsilon) \quad (25)$$

where the electronic stopping konstant k is

$$k = k_L = 0.0793 \left(\frac{Z_1 Z_2}{M_2} \right)^{1/2} \left(\frac{(1+\mu)a}{0.8853a_0} \right)^{3/2} Z_1^{1/6} \quad (26)$$

For the equal mass case we get

$$k \equiv k_2 = 0.133366 Z_2^{2/3} M_2^{-1/2} \quad (27)$$

$$\epsilon_0 \equiv \epsilon_{02} = 11.5034 Z_2^{-7/3} (\text{keV}^{-1}) \quad (28)$$

For $\mu \gg 1$ the Lindhard k is not always in accordance with experimental results. Therefore we introduce a factor k_f so that $k = k_f k_L$ for cases where k has been measured.

The function G(E).

As mentioned above G=0 for the (IR) case. Otherwise G(E) represents the total amount of energy deposited in the specified case (DNE,DEE,DTE)by an ion bombardment in the equal mass situation. For (DTE) it is obvious then that

$$G(E) = E \quad (\text{DTE}) \quad (29)$$

For (DNE), G(E) (normally called $\nu(E)$) has been evaluated by

Sigmund, Matthies and Phillips /12/ and by Robinson /13/. We have here for convenience chosen the Robinson-expression

$$G(E) = E(1+k_2 h(\epsilon_2))^{-1} \quad (\text{DNE}) \quad (30)$$

where
$$h(z) = 3.4008z^{1/6} + 0.40244z^{3/4} + z \quad (31)$$

$\epsilon_2 = \epsilon_{O2} \cdot E$ is E expressed in reduced ($M_2 \rightarrow M_2$) units and k_2 is the corresponding electronic energy loss constant, see (27) and (28).

From (29) and (30) it follows that for (DEE)

$$G(E) = E \frac{k_2 h(\epsilon_2)}{1+k_2 h(\epsilon_2)} \quad (\text{DEE}) \quad (32)$$

For sufficiently small energies we find

$$G(E) = E \cdot \begin{cases} 1 & (\text{DNE}) \quad (30a) \\ 3.4008\epsilon_2^{1/6} k_2 & (\text{DEE}) \quad (32a) \\ 1 & (\text{DTE}) \quad (29a) \end{cases}$$

Method of solution.

In solving the differential equation system (7) it is convenient to introduce dimensionless quantities and to use a scaling which makes it possible to solve the equations analytically in the low energy region. We define

$$f(\epsilon, \bar{e}, \tau) d\tau = F(E, \bar{e}, x) dx \quad (33)$$

$$f^n(\epsilon, \bar{e}) = \int \tau^n f(\epsilon, \bar{e}, \tau) d\tau = \rho_O^n \epsilon_O^{-r} \epsilon^{-p-2mn} F^n(E, \bar{e}) \quad (34)$$

$$f_\ell^n(\epsilon) = \rho_O^n \epsilon_O^{-r} \epsilon^{-p-2mn} F_\ell^n(E) \quad (35)$$

with

$$\tau = x \rho_O \epsilon^{-2m} \quad (36)$$

and
$$f^n(\epsilon, \bar{e}) = \sum_{\ell=0}^{\infty} f_{\ell}^n(\epsilon) P_{\ell}(\cos\theta) \quad (37)$$

Introducing (22), (23), (25) and (35) in (7) yields for $n \neq 0$

$$\begin{aligned} \{s_e(\epsilon) \epsilon^{2m-1} + i_1(\ell, \epsilon)\} \left\{ \epsilon \frac{df_{\ell}^n}{d\epsilon} + (p+2mn) f_{\ell}^n(\epsilon) \right\} \\ + \frac{1}{\gamma} i_2(\ell, \epsilon) f_{\ell}^n(\epsilon) \\ = \frac{n}{2\ell+1} \{ \ell f_{\ell-1}^{n-1}(\epsilon) + (\ell+1) f_{\ell+1}^{n-1}(\epsilon) \} \end{aligned} \quad (38)$$

and for $n=\ell=0$, with

$$s_n(\epsilon) = \frac{\lambda}{2} \epsilon^{1-2m} S(0, \epsilon) = i_1(0, \epsilon) \cdot \epsilon^{1-2m} \quad (39)$$

being the nuclear stopping power in reduced units

$$\begin{aligned} \{s_e(\epsilon) + s_n(\epsilon)\} \left\{ \epsilon \frac{df_0^0}{d\epsilon} + p f_0^0(\epsilon) \right\} \\ = \epsilon_0^{-r-1} \epsilon^{2-p-2m} \frac{\lambda}{2} \int_0^1 y^{-m} (1 + (2\lambda \epsilon^{2-2m} y^{1-m})^q)^{-1/q} \frac{G(T)}{T} dy \\ \equiv \epsilon_0^{-r-1} \epsilon^{1-p} s_{n2}(\epsilon) \end{aligned} \quad (40)$$

where $T = \gamma \epsilon / \epsilon_0$.

Recalling (24a) we get for sufficiently small ϵ and for $m > 1/4$ that the electronic energy loss may be neglected and obtain for $n \neq 0$

$$\begin{aligned} \frac{\lambda}{2} \sum_{k=0}^{2\ell} c_{\ell k} \frac{1}{1+k-m} \epsilon \frac{df_{\ell}^n}{d\epsilon} \\ + \{ (p+2mn) \frac{\lambda}{2} \sum_{k=0}^{2\ell} c_{\ell k} \frac{1}{1+k-m} - \frac{\lambda}{2} \frac{1}{\gamma} \sum_{k=0}^{2\ell-1} c_{\ell, k+1} \frac{1}{1+k-m} \} f_{\ell}^n(\epsilon) \\ = \frac{n}{2\ell+1} \{ \ell f_{\ell-1}^{n-1}(\epsilon) + (\ell+1) f_{\ell+1}^{n-1}(\epsilon) \} \end{aligned} \quad (38a)$$

and for $n=\ell=0$

$$\epsilon \frac{df_0^0}{d\epsilon} + p f_0^0(\epsilon) = \epsilon_0^{-r-1} \epsilon^{1-p} (1-m) \int y^{-m} \frac{G(T)}{T} dy \quad (40a)$$

and using (29a), (30a) and (32a) we see that by a proper choice of p it is possible to make all f_{ℓ}^n constant in this low energy limit

We set

$$\begin{aligned}
 (\text{IR}) & : r=0, p=0 & : f_0^0=1 \\
 (\text{DNE}) & : r=-1, p=1 & : f_0^0=1 \\
 (\text{DEE}) & : r=-1, p=7/6 & : f_0^0=6/7 \cdot 3.4008(\gamma \epsilon_{O2}/\epsilon_O)^{1/6} \cdot \frac{1-m}{7/6-m} k_2 \\
 (\text{DTE}) & : r=-1, p=1 & : f_0^0=1
 \end{aligned} \tag{41}$$

The scaling used here corresponds exactly to the one used in ref.4 where electronic energy loss is neglected over the whole energy range, yielding for a given power cross section a universal function for F in the variable τ .

Generally the summations in (6) and (37) reduces to the range

$$l = n - 2j, \quad j=0, \dots, \frac{n}{2} \tag{42}$$

due to the recursion relations (7) and (38) and the fact that F^0 has no angular dependence.

3. PROGRAM DESCRIPTION .

The following is a detailed description of a program (RADELI) set up to evaluate the moments $F^n(E, \bar{e})$ over the functions F defined in the previous chapter for the special case:

$$\lambda = 1.309, \quad m = 1/3, \quad q = 2/3 \tag{43}$$

For details concerning this choice see ref. /4/, /11/. The region "sufficiently small energies", used in the previous, means in this situation

$$\epsilon \ll k^{-6} \approx \mu^{-6} 10^6 \tag{44}$$

We shall start up with some remarks concerning evaluation of integrals included in the calculations. Apart from the already mentioned ones we shall evaluate the total range which in reduced units is given by

$$\rho_T(\epsilon) = \int_0^\epsilon \frac{d\epsilon}{s_e(\epsilon) + s_n(\epsilon)} \quad (45)$$

With the special values (43) it can be shown that

$$s_n(\epsilon) = \frac{9}{8}\epsilon^{-1} \left\{ \ln(a + \sqrt{1+a^2}) - \frac{a}{\sqrt{1+a^2}} \right\} \quad (46)$$

and we write for convenience with (25)

$$\rho_T(\epsilon) = \int_0^{\sqrt{\epsilon}} \frac{2 dx}{k + \frac{9}{8} x^{-3} \left\{ \ln(a + \sqrt{1+a^2}) - \frac{a}{\sqrt{1+a^2}} \right\}} \quad (47)$$

with $a = (2\lambda)^{1/3} x^{8/9} = (2\lambda)^{1/3} \epsilon^{4/9}$

ρ_T is used for comparison with the mean values F^1/F^0 for nostalgic reasons.

To solve the differential equation system (38) and (40) the integrals i_1 , i_2 and s_{n2} have to be known for arbitrary ϵ . A special procedure is used to reduce computation time at this point. For the special ϵ -values: $\epsilon = j \cdot 10^i$, $j=2,3,\dots,10$, $i=-4,-3,\dots,2$, the integrals are evaluated using a Simpson algorithm. A cubic spline function is assigned to the points and the splines are used to interpolate between the special ϵ -values. The same procedure is used for ρ_T (47). As the functions $S(k,\epsilon)$ (24) are universal, they are evaluated once for all. Further it can be shown that for large k (≥ 8) a Winterbon-formula-approximation to $S(k,\epsilon)$ is very accurate. It takes the form

$$S(k,\epsilon) \approx \frac{\lambda}{2} \frac{1}{k+1-m} \left(1 + \left(2\lambda \frac{k}{k+1-m} \epsilon^{2-2m} \right)^q \right)^{-1/q} \quad (48)$$

From the pre-calculated values of $S(k,\epsilon)$ for $k \leq 7$ and from (48) for $k \geq 8$, $i_1(l,\epsilon)$ and $i_2(l,\epsilon)$ are evaluated using (22) and (23).

D e t a i l l e d d e s c r i p t i o n o f R A D E L I .

(Version moments of range and deposited energies in keV-Å units.
Moments or moments relative to R_T or R_{mean} .)

COMMON blocks used:

/HERB/ AA(12,12), CC(12,25)
/SPEC/ AK,AMY,GAMMA,EPSØ,RHOØ,NMAX,MMAX,NDEF,MART,MREL,LEPS
/SNEPS/ SN,AK22,EPS2Ø,SN2(70,4),EPSMAX,ASN2,NSNT
/INKO/ AI1(12),AI2(12),AKI1(12,70,4),AKI2(12,70,4),E(100),ME
/RTOT/ RT(70,4),UU(100),RMAX,NRTT
/OUTP/ P(8,12),RMEAN(600),ESRCH(100),NR,NUMB,LNUM,NTH,NSRCH

SUBROUTINES used:

HERBI(NMAX)
INIT(NMAX,EPS,C) [C(40)]
FRT(K,EPS,X)
FSN(K,EPS,X)
USIMP(F,K,EPS,A,B,PROC,ISTEP,MSTEP,UD,M)
SPLSMO(N,X,U,Y2,P,A,B,C,D) [X(100),U(100),Y2(100),P(100),A(100),
B(100),C(100),D(100)]
INKOEF(NMAX)
DIFFQ(X,Y,DY) [Y(40),DY(40)]
OUTPUT(EPS,Y,DY,IHLF,MMAX,PRMT) [Y(40),DY(40),PRMT(7)]
DRKGS(PRMT,Y,DY,MMAX,IHLF,DIFFQ,OUTPUT,AUX)
[PRMT(7),Y(40),DY(40),AUX(40,40)]
IBM-SSP subroutine.

Language : FORTRAN

Variable length: REAL(8),INTEGER(4)

Core usage : 240K bites .

S u b r o u t i n e H E R B I (N M A X) .

Evaluates the coefficients $a_{\ell k}$ and $c_{\ell k}$ for $\ell=0,1,\dots,NMAX$;
 $k=0,1,\dots,\ell$, where

$$\begin{aligned}
 P_{\ell}(x) &= \frac{1}{2^{\ell}} \sum_{m=0}^{[\ell/2]} (-)^m \binom{\ell}{m} \binom{\ell-2m}{\ell} x^{\ell-2m} \\
 &= \sum_{k=0}^{\ell} a_{\ell k} x^k
 \end{aligned}$$

see eq.(13) and /14/, and

$$P_{\ell}(\cos\phi') = \sum_{k=0}^{2\ell} c_{\ell k} x^k$$

where

$$\cos\phi' = 1 - 2x + 4/\mu (x-x^2)$$

see eq. (12) and (13).

The value of $\mu=AMY$ is given through /SPEC/ and the values
 $a_{\ell k} = AA(\ell+k,k+1)$ and $c_{\ell k} = CC(\ell+1,k+1)$ are returned through /HERB/.

Method:

$a_{\ell k}$ is evaluated using the recursion scheme

$$a_{\ell\ell} = \frac{1}{2} \frac{(2\ell)!}{\ell! \ell!}$$

and

$$a_{\ell, \ell-2(m+1)} = a_{\ell, \ell-2m} \frac{(\ell-2m-1)(\ell-2m)(-)}{(2\ell-2m-1)(m+1) 2}$$

$$a_{\ell, \ell-2m-1} = 0 \quad , \quad m=0,1,\dots, [\ell/2] - 1$$

$c_{\ell k}$ is evaluated using

$$\sum_{k=0}^{2\ell} c_{\ell k} x^k = \sum_{k=0}^{\ell} a_{\ell k} (\alpha + \beta x + \delta x^2)^k$$

$$= \sum_{k=0}^{\ell} a_{\ell k} \alpha^k \sum_{j=0}^k \binom{k}{j} \left(\frac{\beta}{\alpha}\right)^j \sum_{i=0}^j \binom{j}{i} \left(\frac{\delta}{\beta}\right)^i x^{i+j}$$

where

$$\binom{j}{i} = \frac{j!}{i! (j-i)!} \equiv B(j+1, i+1)$$

$j=0, 1, \dots, NMAX, i=0, 1, \dots, j,$

is determined using

$$\binom{j}{0} = \binom{j}{j} = 1 \text{ and } \binom{j}{i} = \binom{j-1}{i-1} + \binom{j-1}{i}$$

for $0 < i < j$; $\alpha = 1$, $\beta = -2 + 4/\mu$ and $\delta = -4/\mu$.

S u b r o u t i n e I N I T (N M A X , E P S , C) .

Evaluates f_{ℓ}^n in the "sufficiently small energy" regions where they are constant, using the formulae (38a) and (41). The value of $\gamma = 4 \cdot \text{GAMMA}$ and $3.4008 (\gamma \epsilon_{O2} / \epsilon_O)^{1/6} \frac{1-m}{776-m} k_2 = \text{ASN2}$ are transferred through /SPEC/ and /SNEPS/. EPS is a dummy variable. f_{ℓ}^n are returned through the parameter C(i) where only those f_{ℓ}^n not trivial equal zero are stored in the following order:

$$f_0^0, f_1^1, f_0^2, f_2^2, f_1^3, f_3^3, f_0^4, f_2^4, f_4^4, \dots$$

F u n c t i o n F R T (K , E P S , X) .

Evaluates

$$\text{FRT}(X) = 2 \left\{ k + \frac{9}{8} X^{-3} \left(\ln(a + \sqrt{1+a^2}) - \frac{a}{\sqrt{1+a^2}} \right) \right\}^{-1}$$

where

$$a = (2\lambda)^{1/3} X^{8/9}, \text{ for } X \geq 10^{-3}$$

and
$$FRT(X) = 2 \{ k+3/4 X^{-1/3} \}^{-1} \text{ for } X < 10^{-3}$$

The value of k=AK is transferred through /SPEC/.

FRT is used for evaluation of the total range ρ_T . See eq. (47).

K and EPS are dummy variables.

F u n c t i o n F S N (K , E P S , X) .

Evaluates the function

$$FSN(EPS,X) = (1 + (2\lambda EPS^{2-2m} X)^q)^{-1/q} (1 + k_2 h(\gamma \cdot EPS \cdot \epsilon_{O2} / \epsilon_O X^{\frac{1}{1-m}}))^{-1}$$

The values of $\gamma \epsilon_{O2} / \epsilon_O = EPS2\emptyset$ and $k_2 = AK22$ are transferred through /SNEPS/.

FSN is used for evaluation of the integral s_{n2} . K is a dummy var.

S u b r o u t i n e U S I M P (F , K , E P S , A , B , P R O C , I S T E P , M S T E P , U D , M) .

Evaluates the integral

$$UD = \int_A^B F(x, EPS) dx$$

using a Simpson method with automatic step halving until, with M steps, an accuracy better than PROC percent is reached. The interval [A,B] is initially divided in ISTEP subintervals and UD is returned to the calling program when the wanted accuracy is reached or when the number of steps exceeds MSTEP. K is a dummy variable.

S u b r o u t i n e S P L S M O (N , X , U , Y 2 , P , A , B
C , D) .

Evaluates the $4N-4$ spline coefficients A,B,C,D to N given points (X,U). The actual routine is a smoothing spline procedure using the N weights P. Y2 is a working storage. SPLSMO is described in ref /15/.

The value of the spline function is

$$A(n) z^3 + B(n) z^2 + C(n) z + D(n)$$

for $x \in [X(n), X(n+1)]$ and with $z=x-X(n)$.

S u b r o u t i n e I N K O E F (N M A X) .

Manages the evaluation of the coefficients A(I),B(I),C(I),D(I), I=1,...,63 in the cubic spline approximation corresponding to the energy intervals $E(I) = j \cdot 10^i$, $i=-4, \dots, 2$, $j=2, \dots, 10$ for the functions

$$s_{n2}, \rho_T, i_1(\ell, \epsilon) \text{ and } i_2(\ell, \epsilon)$$

Further, the constant values of $i_1(\ell)$ and $i_2(\ell)$ for small energies are calculated. (22), (23), (24) and (24a).

The values of s_{n2} and ρ_T in E(I) are directly evaluated by integration (USIMP,FSN and FRT). i_1 and i_2 are evaluated in E(I) using the formulae (22) and (23).

For $k=0, \dots, 7$ the values of $S(k, \epsilon)$ in E(I) are precalculated and read in. For $k=8, \dots, 2 \cdot NMAX$ $S(k, \epsilon)$ is evaluated using (48).

The coefficients A,B,C,D,renamed 1,2,3,4 (parameter J),in the point E(I) are stored in

s_{n2} : SN2(I,J) /SNEPS/
 ρ_T : RT(I,J) /RTOT/
 $i_1(\ell, \epsilon)$: AKI1($\ell+1$,I,J) /INKO/
 $i_2(\ell, \epsilon)$: AKI2($\ell+1$,I,J) /INKO/
 $i_1(\ell, \epsilon \ll 1)$: AI1($\ell+1$) /INKO/
 $i_2(\ell, \epsilon \ll 1)$: AI2($\ell+1$) /INKO/

E(I) is returned through /INKO/ together with the max value of I : Kl.

S u b r o u t i n e D I F F Q (X , Y , D Y) .

Evaluates,for given values of $Y=f_{\ell}^n$ and $X=\epsilon$,the differential quotient defined by eq. (38) and (40)

$$\frac{df_{\ell}^n}{d\epsilon} = DY$$

$n=0, \dots, NMAX$, $\ell=0, \dots, n$.

The values are given and returned through Y,X and DY in the sequence given in INIT. F. ex. $f_{\ell}^n = Y(M)$ where

$$M = \left[\frac{\ell+2}{2} \right] + \left[\frac{n+1}{2} \right] \cdot \left[\frac{n+2}{2} \right]$$

where all the divisions are integer evaluated.

The start values are given from the INIT program and are evaluated according to eq. (38a), (40a) and (41).

For sufficiently small ϵ the equations (38a) and (40a) are used otherwise equations (38) and (40) are used.

Further DIFFQ evaluates $s_n=SN$ and $\rho_T=RMAX$ in X, these values are returned through /SNEPS/ and /RTOT/.

S u b r o u t i n e O U T P U T (E P S , Y , D Y , I H L F ,
M M A X , P R M T) .

Output routine managing the different modes of output.

EPS,Y,DY,IHLF are returned from the differential equation solver DRKGS, EPS being the actual energy, Y and DY the corresponding values of f_{ℓ}^n and $\frac{df_{\ell}^n}{d\varepsilon}$ and IHLF specifies the number of subsections of the initial interval of solution (see description of RKGS /16/), MMAX the total number of evaluated functions f_{ℓ}^n (the dimension of Y and DY) and PRMT contains 7 parameters specifying the interval (see MAIN program).

The routine writes subheadings on each second page of output and write for each of the NSRCH specified energies ESRCH an output subsection for that EPS for which $|\text{EPS}-\text{ESRCH}| \leq \text{ESRCH} \cdot 10^{-3}$ or if NSRCH=0 for the energies $j \cdot 10^i$ (keV), $j=10,11,\dots,100$, $i=-4,-3,\dots,1$.

Each output subsection consists of NTH lines, one for each of the specified bombardment angles THETA. If NTH=0 only one line for THETA=0 is printed.

NSRCH,ESRCH(i),NTH and $P_{\ell}(\cos(\text{THETA}(j))) = P(j,\ell+1)$ are transferred through /OUTP/.

The different modes of output are specified by NDEF, MART, MREL /SPEC/ :

- NDEF=0 gives (IR) output,
- NDEF=1 gives (DNE) output,
- NDEF=2 gives (DEE) output,
- NDEF=3 gives (DTE) output.

MART =0 results in the following output line :

energy E, $F^n(E, \text{THETA})$, $n=0, \dots, \text{NMAX}$, $S(E)$, where S is S_n for (IR) and (DNE), S_e for (DEE) and $S_n + S_e$ for (DTE).

MART=1 results in :

for NDEF=0

E, RTOT, MEAN, SIGM, MEAN/RTOT, STRAGREL, SKEWNESS, KURTOSIS, EPS

for NDEF=1,2,3 and MREL=0

E, EFRACT, MEAN, SIGM, MEAN/RTOT, STRAGREL, SKEWNESS, KURTOSIS, EPS, S

for NDEF=1,2,3 and MREL=1

E, EFRACT, MEAN, SIGM, MEAN/RMEAN, STRAGREL, SKEWNESS, KURTOSIS, EPS, S

where E is the energy, RTOT the total range, EPS is the ϵ corresponding to E, S is as defined above and RMEAN is MEAN for NDEF=0, or the mean range. The left parameters are all taken in E and are defined as follows :

$$\begin{aligned} \text{EFRACT} &= F^0/E \\ \text{MEAN} &= F^1/F^0 \\ \text{SIGM} &= \sqrt{F^2/F^0 - (\text{MEAN})^2} \\ \text{STRAGREL} &= (\text{SIGM}/\text{MEAN})^2 \\ \text{SKEWNESS} &= (F^3/F^0 - 3F^2/F^0 F^1/F^0 + 2(F^1/F^0)^3) / (\text{SIGM})^3 \\ \text{KURTOSIS} &= (F^4/F^0 - 4F^3/F^0 F^1/F^0 + 6F^2/F^0 (F^1/F^0)^2 - 3(F^1/F^0)^4) / (\text{SIGM})^4 \end{aligned}$$

All parameters are primarily evaluated in reduced units ϵ , ρ , ρ_T , s , f^n . For LEPS#R (in MAIN program) these are transformed to (keV-Å) units using $E=\epsilon/\epsilon_0$, $x=\rho/\rho_0$, (34) and (41).

MAIN program.

Reads in specification values and controls the calls of sub-routines.

First data card read :

IDENTIFICATION= up to 72 letters or numbers used for the heading printed on the first side of output.

Second data card read :

Z1=Z₁, AM1=M₁, Z2=Z₂, AM2=M₂, D2=N in g/cm³, NSRCH=number of output energies wanted, NTH=number of bombardment angles wanted, LF=parameter for choice of Lindhard a_L (L) or Firsov a_F (F) (see eq.(20L) and (20F), FAKTOR= factor on the Lindhard value of k in the electronic stopping (eq.(25) and (26)) k_f, LEPS= parameter for output in keV-Å units (blank) or reduced units ($\epsilon=\epsilon_0 E$, $\rho=\rho_0 x$) (R).

Third data card read :

NART=parameter specifying moments (M) or relative moments (R) for output. NREL=parameter specifying (for deposited energies only) relativity to total range (T) or to mean range (M). For NART=M,NREL is dummy, NARTand NREL are separated by a dummy character. NMAX= the maximum order of moments to be evaluated, for NART=R NMAX is set to 4,

NSORT= up to 4 letter pairs separated by commas specifying the deposition modes : RA=(IR), EN=(DNE), EE=(DNE), ET=(DTE).

Fourth input card read :

THETA(I), I=1,...,NTH, values of bombardment angles (degrees).

For NTH=0 THETA(1) is set to 0 and NTH to 1.

Following input cards read :

ESRCH(I), I=1,...,NSRCH, values of the wanted output energies in keV for LEPS=blank and in reduced units for LEPS=R. For NSRCH=0 standard values are used, see OUTPUT.

On the basis of the input values μ , γ , ϵ_0 , ϵ_{02} , k_2 , ρ_0 and k are evaluated and printed in a heading together with the IDENTIFICATION.

$P_\ell(\cos(\text{THETA}(i))) = P(i, \ell+1)$ is evaluated using AA /HERB/ according to eq. (13), for $i=1, \dots, \text{NTH}$ and $\ell=0, \dots, \text{NMAX}$.

The differential equation solver DRKGS is called with initial intervals $[10^j \epsilon_0 - 10^{j+1} \epsilon_0]$, $j=-9, \dots$ divided initially in 100 subintervals. The values of the start and end of intervals and the length of subintervals are transferred through PRMT(1,2,3). PRMT(4) is the sum of acceptable error on the evaluated f_ℓ^n , and is here chosen to be $\leq 10^{-4}$ max. for each. This is done by proper choice of PRMT(4) and the initial value of DY, see description of DRKGS /16/ for details.

A warning is given if the wanted accuracy is not reached within 10 halvings of the subintervals, the warning contains NDEF, PRMT(1) and IHLF, the error parameter of DRKGS.

The program terminates the solution procedure at $\epsilon = 10^3$ or at the largest given ESRCH value less than $10^3 \epsilon/\epsilon_0$.

L i m i t a t i o n s a n d r e s t r i c t i o n s .

Max number of given output energies (ESRCH) 100.

Max number of bombardment angles (THETA) 8.

Max order of evaluated moments (NMAX) 11.

The values of $\frac{\lambda}{2} S(k, \epsilon)$ for $k=0, \dots, 7$ and $\epsilon=i \cdot 10^j$, $i=2, \dots, 10$ $j=-4, \dots, 2$ has to be supplied before the mentioned data cards, one ϵ on each card with format (8D9.4).

Compilation time : 12 sec.

Execution time : 1 min per (IR), (DNE), (DEE), (DTE)
on an IBM 360/91

Examples of input cards to MAIN program, indicating the fixed formats used:

1. |IDENTIFICATION-FIELD, MAX 72 CHARACTERS. →
2. |000.00|00.00|00.00|00.00|00.00|00.00|00.00|00.00|
3. |A| |A|00|,|AA|,|AA|,|AA|,|AA|
4. |000.00|00.00|00.00|00.00|00.00|00.00|00.00|00.00|00.00|
- 5a. |0000.0000|0000.0000|0000.0000|0000.0000|0000.0000|
| ... |0000.0000|0000.0000| ... |
- 5b. - " -
- .
- .
- .

2. | 1.00 2.00 6.00 12.00 2.35 102L 2.13

Bombardment D → C, 10 energies and 2 angles, factor 2.13 to the Lindhard k, and Lindhard scaling (a_L) used.

2. | 1.00 2.00 6.00 12.00 2.35 102F R

Same but with Firsov scaling, factor 1 and in reduced units.

3. | MOM07,RA,ET,EN

Moments F^0, \dots, F^7 of (IR), (DNE), and (DTE).

3. | RMT ,EE,EN,RA

Moments relative to total range (max 4) of (IR), (DNE), and (DEE).

3. | RMM ,EE,EN,ET,

Moments relative to mean range (max 4) of (DNE), (DEE), and (DTE).

4. | 90.00 .25 0.00

Values of THETA, NTH must be specified to 3 in this case.

5. | 0.015 150.0000

Values of output energies, NSRCH here 2.

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