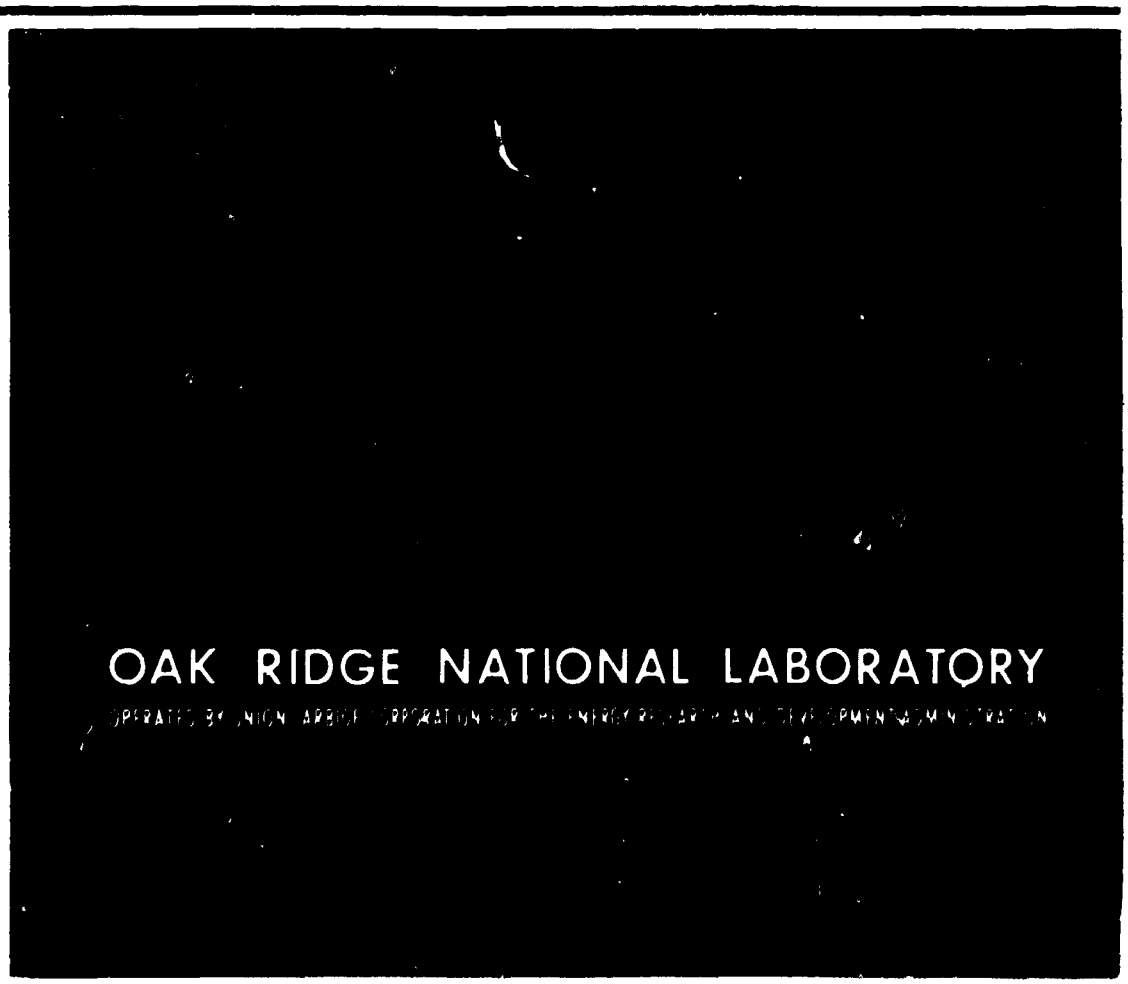
ORNL/CSD/TM-2

SWIMS
A Small-Angle Multiple Scattering Computer Code

R. O. Sayer



OAK RIDGE NATIONAL LABORATORY

OPERATED BY UNION CARBIDE CORPORATION FOR THE ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

BLANK PAGE

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 $4.00; Microfiche $2.25

3.5

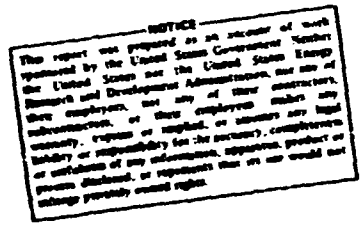
ORNL/CSD-TM-2

Contract No. W-7405 eng 26

COMPUTER SCIENCES DIVISION

SWIMS
A Small-Angle Multiple Scattering Computer Code

R. O. Sayer



JULY 1976

UNION CARBIDE CORPORATION, NUCLEAR DIVISION
operating the
Oak Ridge Gaseous Diffusion Plant . Oak Ridge National Laboratory
Oak Ridge Y-12 Plant . Paducah Gaseous Diffusion Plant
for the
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

TABLE OF CONTENTS

ACKNOWLEDGMENTS

The author is pleased to acknowledge enlightening discussions with W. T. Milner and C. M. Jones of the Physics Division.

ABSTRACT

SWIMS (Sigmund and Winterbon Multiple Scattering) is a computer code for calculation of the angular dispersion of ion beams that undergo small-angle, incoherent multiple scattering by gaseous or solid media. The code uses the tabulated angular distributions of Sigmund and Winterbon[1] for a Thomas-Fermi screened Coulomb potential. The fraction of the incident beam scattered into a cone defined by the polar angle α is computed as a function of α for reduced thicknesses over the range $0.01 \leq r \leq 10.0$.

I. INTRODUCTION

Energetic heavy ion beams emerge from gases and thin foils with angular spreads that are of considerable practical interest for design of accelerators and experimental apparatus. Meyer[2] has developed a theory that predicts the angular distribution of particles that undergo multiple scattering in thin foils at small angles. Recently Sigmund and Winterbon[1] (hereafter referred to as SW) reevaluated Meyer's distributions with more accurate numerical procedures and extended the range of reduced thickness, r.

SW find excellent agreement with Meyer's distributions out to twice the half-width, but there are substantial differences in the tails of the distributions, particularly for small r. They attribute the discrepancies to lack of accuracy in Meyer's numerical procedures.

Some quantities needed for use of the computer code are defined below, and others are defined in the Appendix. For a more complete treatment Meyer[2] and SW may be consulted.

$F(t,\alpha)\, d\Omega$ = angular distribution of a particle beam after traversing a thin layer.

α = total deflection angle.

BLANK PAGE

$d\Omega$ = solid angle corresponding to α.

t = penetrated depth.

The distribution function is normalized so that

$$\int F(t,\alpha)\, d\Omega = 2\pi \int_0^\infty \alpha\, d\alpha\, F(t,\alpha) = 1 \quad . \tag{1}$$

By changing to dimensionless variables r and $\tilde{\alpha}$, the distribution may be written

$$F(t,\alpha)\, d\Omega \equiv \tilde{\alpha}\, d\tilde{\alpha}\, f_1(r,\tilde{\alpha}) \quad . \tag{2}$$

The reduced thickness r is given by

$$r = \pi a^2 N t \tag{3}$$

where

a = screening radius,

N = number of scattering centers unit volume.

The reduced scattering angle $\tilde{\alpha}$ is given by

$$\tilde{\alpha} = \alpha\, E a\, [2Z_1 Z_2 e^2] \tag{4}$$

where

E = projectile energy,

Z_1 = projectile atomic number,

Z_2 = target atomic number,

e = electronic charge.

SW note that, for very thin foils:

$$\lim_{x \to 0} F(x,\alpha)\, d\Omega = Nx\, d\sigma(\alpha) \tag{5}$$

where $d\sigma(\alpha)$ is the single-scattering distribution.[3]

SW have evaluated $f_1(\tau,\tilde{\alpha})$ for selected τ and $\tilde{\alpha}$ values. Their tabulated f_1 values are used in the present SWIMS code to compute the quantity

$$FINT(\tau,\tilde{\alpha}) = \int_0^{\tilde{\alpha}} \tilde{\alpha}\, d\tilde{\alpha}\, f_1(\tau,\tilde{\alpha}) \tag{6}$$

which may be interpreted as the fraction of the scattered beam contained within the cone defined by the half-angle $\tilde{\alpha}$. From Eq. (1) we see that

$$\lim_{\tilde{\alpha} \to \infty} FINT(\tau,\tilde{\alpha}) = 1 \quad . \tag{7}$$

Usually the behavior of the integral FINT is of more interest in accelerator applications than the distribution f_1. Therefore, both FINT and f_1 are computed as a function of α by SWIMS for arbitrary thickness in the range $0.01 \leq \tau \leq 10.0$. Alternately, the angles corresponding to specified fractions of the scattered beam may be computed for specified target thicknesses.

For computational convenience we define new variables

$$\delta \equiv \tilde{\alpha}\, \tilde{\alpha}_{1/2} \; ; \tag{8}$$

$$f_1(\tau,\tilde{\alpha}) = f_1(\tau,0)\, f_d(\tau,\delta) \tag{9}$$

where

$\tilde{\alpha}_{1/2}$ = half-width at half-maximum of the distribution

Then Eq. (6) becomes

$$FINT(\tau,\delta) = (\tilde{\alpha}_{1/2})^2\, f_1(\tau,0) \int_0^{\delta} \delta\, d\delta\, f_d(\tau,\delta) \quad . \tag{10}$$

II. PROCEDURE

A third-order polynomial in ln τ for ln $\tilde{\alpha}_{1:}$ was fit[4] to the $\tilde{\alpha}_{1:}$ values obtained by interpolation from the SW tables of $f_1(\tau,\alpha)$. The SW tables were converted with the aid of Eq. (9) to tables of δ and $f_d(\tau,\delta)$ for τ = 0.01, 0.05, 0.1, 0.2, 0.4, 0.6, 1.0, 2.0, 10.0. Weighted least squares fits[4] of polynomials in δ to ln $f_d(\tau,\delta)$ were performed with weights proportional to the product $\delta \cdot f_d$, i.e. to the integrand in Eq. (10). The coefficients from the fits are used by SWIMS to compute the integral FINT(τ,δ). Interpolation of ln f_d on ln τ for a given value of δ is employed to obtain f_d for τ values intermediate to the tabular values. Since the quantity $(\tilde{\alpha}_{1:})^2 f_1(\tau,0)$ in Eq. (10) varies smoothly from 0.233 to 1.054 over the range $0.01 \leq \tau \leq 10.0$, linear interpolation on τ is sufficient.

The $\tilde{\alpha}_{1:}$ values were fit to 0.6% or better over the range $0.02 \leq \tau \leq 160.$, and the $f_d(\tau,\delta)$ values were fit to 2% or better over the entire range of δ values for which the integrand $\delta \cdot f_d$ was significant. For most δ values the tabular and fit f_d values agreed to better than 1%. The interpolation procedures are thought not to introduce errors larger than 2%. Thus the f_d values computed by SWIMS are felt to represent, for $0.02 \leq \tau \leq 10.0$, the corresponding $f_1(\tau,\tilde{\alpha})$ functions of SW to accuracies of 3-4% or better. Of course FINT is determined to higher precision than f_d since the integration produces some smoothing. As a check Eq. (10) was evaluated for large δ with the following results:

τ	FINT($\tau,\delta\to\infty$)
0.4	0.987
1.0	0.991
2.0	0.993
5.0	1.014
10.0	1.005

The FINT($\tau,\tilde{\alpha}$) values for selected τ values were interpolated to obtain $\tilde{\alpha}$ values corresponding to 40%, 60%, and 80% of the scattered beam, and the results are displayed in Fig. 1. Corresponding

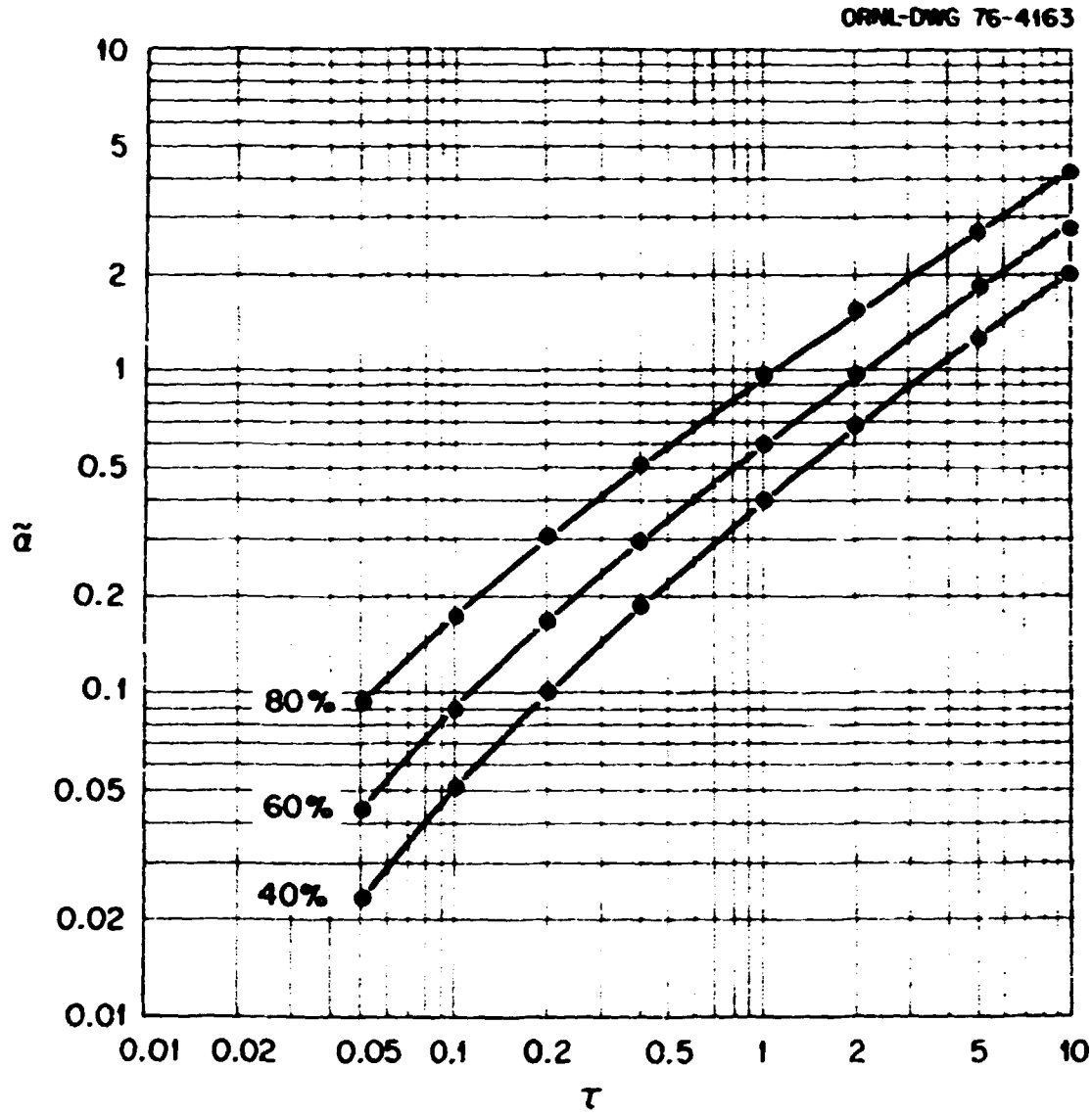


Fig. 1. Plot of reduced angle $\tilde{\alpha}$ versus reduced thickness τ. The angle $\tilde{\alpha}$ specifies a cone that contains the indicated percentage of the incident beam intensity.

α and ρt values may be computed with the aid of numerical formulas in the following section. However, it is much easier to let SWIMS do the calculations as outlined in the Appendix.

III. NUMERICAL FORMULAS AND DEFINITIONS

The screening radius a is given by

$$a = (0.885 a_o) \cdot [(Z_1^{2/3} + Z_2^{2/3})^{1/2}]$$

where $a_o = 0.529 \times 10^{-8}$ cm.

The collision diameter b is given by

$$b = (2 Z_1 Z_2 e^2)(1 + A_1/A_2)/(m_1 v^2)$$

$$= 1.4398 \times 10^{-13}(1 + A_1/A_2) Z_1 Z_2 / E \text{ cm},$$

where E = projectile energy in MeV, and A_1 and A_2 are the projectile and target masses, respectively. The reduced energy ϵ is defined by the relation

$$\epsilon = a/b .$$

and half the distance between neighboring atoms is given by $r_o = 0.5/N^{1/3}$. The average number of collisions in a layer of thickness t is given by

$$NUM = \pi r_o^2 Nt .$$

Let

$$\rho = \text{density in mg/cm}^3$$

$$\rho t = \text{thickness in } \mu\text{g/cm}^2.$$

Then

$$Nt = 6.023 \times 10^{17}\ \rho t / A_2 \quad \text{atoms/cm}^2$$

and

$$\tau = (41.473 \rho t) / [A_2(Z_1^{2/3} + Z_2^{2/3})] \quad .$$

Also we note that

$$\tilde{\alpha} = \alpha (1 + A_1/A_2)\ \epsilon/2$$

$$\tilde{\alpha} = \alpha (16.258.E) / [Z_1 Z_2 (Z_1^{2/3} + Z_2^{2/3})^{1/2}] \quad .$$

REFERENCES

1. P. Sigmund and K. B. Winterbon, "Small-Angle Multiple Scattering of Ions in the Screened Coulomb Region," Nucl. Inst. Meth. 119, 541 (1974).

2. L. Meyer, "Plural and Multiple Scattering of Low-Energy Heavy Particles in Solids," Phys. Stat. Sol. 44, 253 (1971).

3. J. Lindhard, V. Nielsen, and M. Scharff, "Approximation Method in Classical Scattering by Screened Coulomb Fields," Kgl. Danske Videnskab. Selskab., Mat.-Fys. Medd. 36, No. 10 (1968).

4. Linear least-squares fits were performed with FUNKYFIT, a routine written by W. T. Milner.

APPENDIX: SWIMS USER NOTES

There are two modes of operation: one-shot and table specified by 1 and 2, respectively, punched in column 1 of the MODE card. Sample outputs are given at the end of this section, and a discussion of the input and program operation follows.

Two versions of SWIMS exist; one for PDP-10 users and one for CDC-3200 (Bldg. 5500) users.

To run the CDC-3200 version, prepare the input data cards as described below and read in the SWIMS control deck with data cards.

To run the PDP-10 version, log on and type the command: .FILE R. D647. SWIMS.REL. When the file has been read from dectape, type .EX SWIMS.REL. Then input data in a conversational manner (in 8F format). In the 'one-shot' mode, values of FINT are typed every 10^{th} integration step and written on a file called MEYER.DAT every 2^{nd} step. In the 'TABLE' mode output is both to the user's terminal and to a file called TABLE.DAT.

MODE = 1 (One-Shot) Operation

A sample data deck is shown below. Z1 and A1 are the projectile atomic number and mass; Z2 and A2 are the target atomic number and mass. E is the projectile energy in MeV. RHOT is the target thickness in $\mu g\ cm^{-2}$. RHO is the target density in $gm\ cm^{-3}$. PPLOT $\neq$ 0 produces a line printer plot of FINT versus δ. Default values: RHOT = 1.0$\mu g\ cm^{-2}$, RHO = 1.88 $gm\ cm^{-3}$.

The series of 'E' cards ends with a blank card that causes a new 'AZ' card to be read. Two adjacent blank cards end the sequence and cause a new 'MODE' card to be read. A blank MODE card terminates the program.

MODE	card	1 (I1)
AZ	card	Z1, A1, Z2, A2 (4F8.0)
E	card	E, RHOT, RHO, PPLOT (4F8.0)
⋮		
blank	card	
AZ	card	
E	card	
⋮		
blank	card	
blank	card	
MODE	card	

etc.

MODE = 2 (Table) Operation

A sample data deck is shown below. The 'FRAK' card contains the FRACT array, whose default values are 0.2, 0.4, 0.6, 0.8, 0.9. For each ρt value specified by the 'ρt' card, SWIMS performs a MODE 1 type calculation to obtain the FINT(τ,α) array which is interpolated to obtain an α value for each beam fraction specified by FRACT. [See Eq. (6).] A table of α values versus ρt values is printed.

On the 'ρt' card the number, RONUM, may be used to specify up to ten ρt values equally spaced between ρt_{min} and ρt_{max}, in units of $\mu g \cdot cm^{-2}$. However, if ρt_{min} is set to zero, the program will choose ρt values that span the range of reduced thickness $0.01 \leq \tau \leq 10.0$. This option was used to produce the sample output.

As in MODE 1 operation, one blank causes a new 'AZ' card to be read, and two adjacent blanks cause a new 'MODE' card to be read.

MODE	card	2 (I1)
AZ	card	Z1, A1, Z2, A2 (4F8.0)
FRAK	card	FRACT array (5F8.0)
E	card	E (F8.0)
ρt	card	ρt_{min}, ρt_{max}, RONUM (3F8.0)
E	card	
ρt	card	
blank	card	
AZ	card	
FRAK	card	
E	card	
ρt	card	
blank	card	
blank	card	
MODE	card	

etc.

SYMBOL - FORTRAN EQUIVALENCES

Symbols	FORTRAN Names
Z_1, A_1, Z_2, A_2	Z1, A1, Z2, A2
E	E
ρt, ρ	RHOT, RHO
τ	TAU
r_0, NUM	RO, NUM
a, b, ϵ	A, B, EPS
$\alpha_{1,2}$	GI or AWIG 1 2
$\alpha_{1/2}$	THALF or ALP 1 2
δ	DELTA
$\tilde{\alpha}$	AWIG or TWIG
α	ALPHA or THETA
$f_\delta(\tau,\delta)$	FD or FI
FINT(τ,δ)	FINT

SWIMS MODE=1 OUTPUT

Z1	A1	Z2	A2	E (MEV)	RHOT UG/CM**2	RHC GM/CM**3
8.	16.	18.	40.	25.00	1.000	1.880

RO (CM)	N	A (CM)	B (CM)	EPS	TAU	G1	T 1/2 (MRAD)
1.64E-08	1.27E+01	1.42E-09	1.16E-12	1.22E+03	0.09540	0.01969	0.02300

L	DELTA	ANIG	ALPHA	FD	FINT
1	0.00	0.0000	0.000	1.00000	0.0000
11	1.00	0.0197	0.023	0.50075	0.1384
21	2.00	0.0394	0.046	0.20320	0.3280
31	3.00	0.0591	0.069	0.09888	0.4702
41	4.00	0.0788	0.092	0.05352	0.5722
51	5.00	0.0984	0.115	0.03184	0.6469
61	6.00	0.1181	0.138	0.02003	0.7030
71	7.00	0.1378	0.161	0.01345	0.7461
81	8.00	0.1575	0.184	0.00935	0.7800
91	9.00	0.1772	0.207	0.00672	0.8071
101	10.00	0.1969	0.230	0.00500	0.8293
111	11.00	0.2166	0.253	0.00385	0.8479
121	12.00	0.2363	0.276	0.00306	0.8638
131	13.00	0.2559	0.299	0.00251	0.8778
141	14.00	0.2756	0.322	0.00210	0.8904
151	15.00	0.2953	0.345	0.00187	0.9020

SWIMS MODE=2 OUTPUT

SIGMUND & WINTERBON MULTIPLE SCATTERING, NIM 119, 541.

Z1	A1	Z2	A2	E/MEV
8.	16.	18.	40.	25.00

TAU	RBOT	ANG1/2	ALP1/2	--- ANGLES IN HEAD FOR BEAM FRACTIONS: --				
				0.20	0.40	0.60	0.80	0.90
0.010	0.105	0.001	0.001	0.002	0.003	0.008	0.000	0.000
0.050	0.524	0.008	0.009	0.014	0.028	0.051	0.111	0.000
0.100	1.048	0.021	0.025	0.032	0.059	0.104	0.205	0.386
0.200	2.096	0.053	0.061	0.066	0.119	0.196	0.361	0.593
0.400	4.193	0.120	0.140	0.130	0.221	0.348	0.602	0.981
0.600	6.289	0.186	0.217	0.186	0.312	0.479	0.804	1.229
1.000	10.482	0.306	0.358	0.286	0.468	0.704	1.182	1.699
2.000	20.965	0.565	0.660	0.491	0.789	1.157	1.810	2.615
5.000	52.411	1.177	1.375	0.951	1.501	2.185	3.209	4.402
10.000	104.823	1.955	2.283	1.521	2.382	3.362	4.982	6.695