Report #1

APPLIED PHYSICS DIVISION

PHYSICS REPORT

PLASMA PHYSICS LABORATORY

DISTRIBUTION OF NEUTRALS SCATTERED OFF A WALL

GLENN BATEMAN

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DISTRIBUTION OF NEUTRALS SCATTERED OFF A WALL

BY

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The distribution of scattered neutral atoms is computed as a function of scattered velocity, polar angle, and azimuthal angle for a range of incident energies and polar angles using the MARLOWE computer code, for deuterium scattered off stainless steel with a smooth surface and amorphous substrate. Using inverse cumulative distributions, the results are expressed in a way that can be used directly in Monte Carlo codes which follow atoms and ions that strike material walls. The transition from the forward peaked distribution at normal incidence to nearly specular reflection at grazing incidence is studied.

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Distribution of Neutrals Scattered off Wall

Energetic ions and atoms striking a material wall have a probability of scattering off the wall or of becoming imbedded within the wall. Under steady-state conditions, the particles imbedded in the wall generally diffuse to the surface and are reemitted as neutral atoms or molecules with energy comparable to the wall temperature. The scattered particles generally transfer some of their momentum and energy to the wall and return as neutral atoms. The nature of the scattering process has attracted increased attention as more research has been done on plasma-wall interactions in controlled thermonuclear fusion experiments.

In particular, Monte Carlo codes such as BALDUR and DEGAS at Princeton which consider individual ions and atoms incident on a wall, need to be given a specific prescription for the distribution of scattered particles in energy and angle. To date, ad hoc prescriptions have been used which agree qualitatively with some of the features of computed and experimentally observed scattered distributions. In order to improve on this situation, I have used the MARLOWE code from Dr. Mark Robinson to compute and tabulate the detailed scattering distribution for deuterium incident on an amorphous steel (Fe) wall with a smooth surface. The data has been tabulated for incident angles α = 0°, 20°, 40°, 60°, and 80° relative to the normal and incident energies 50 eV, 100 eV, 200 eV, 500 eV, and 1 keV. The procedure has been standardized and automated for use with other incident particles (tritium, helium, impurities, ...) and other wall substrates (such as carbon, aluminum, copper, ...). Some of the data has been checked against results of the TRIM code provided by Dr. Lee Haggmark (Sandia, Livermore) and against both computed and experimental results presented in the literature.

The MARLOWE and TRIM Codes

Both the MARLOWE and TRIM codes use Monte Carlo techniques to simulate the motion of the incident particle through a solid substrate. The motion is influenced by three effects (Eckstein, Verbeek and Biersack, J. Appl. Phys. 51, (1980) 1194).

(1) Angular scattering off substrate atoms approximated by a Molière repulsive potential. The MARLOWE code considers some simultaneous collisions with a cutoff parameter.[1] Since the potential is purely repulsive, there is no possibility for chemical absorption or surface sticking. Some of these approximations are believed to break down at low energy (≤ 50 eV).

(2) There is slowing down off the electrons in the substrate (see H. H. Anderson and J. F. Ziegler "Hydrogen Stopping Power and Ranges in All Elements," Pergamon Press, New York, 1977).

(3) There is also energy loss to the substrate ions (see O.S. Oen and M. T. Robinson, J. Nucl. Mater. 76-77, 370, 1978).

The MARLOWE code can be run with a single crystal substrate (Poly = .F., .F.) or a "poly-crystaline" substrate (Poly = .T., .F. which gives a single randomly chosen rotation to the crystal just once before each incident particle is launched) or as an "amorphous" solid (Poly = .T., .T. which makes a random rotation between each collision).

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[1] Note: I have set RB = 0.42, 0.42 as the cutoff parameter in MARLOWE following Robinson's advice.

I have consistently used the "amorphous" option.

The MARLOWE code is well documented (National Energy Software Center, Argonne Code Center, Access #680) and available on the MFE computer center. The version I had access to needed to be compiled under LASLFTN (see Appendix I).

The TRIM code considers a truely amorphous substrate. It is shorter and faster. TRIM is not yet available on the MFE computer. Dr. L. Haggmark provided copies of the output for a series of runs with

$$\left\{\begin{matrix} D \\ He \end{matrix}\right\} \rightarrow \left\{\begin{matrix} Fe \\ C \end{matrix}\right\} \qquad \begin{matrix} E = 50 \text{ eV}, 100 \text{ eV} \\ \alpha = 0^\circ, 20^\circ, 40^\circ, 60^\circ, 80^\circ. \end{matrix}$$

As noted in the reference list, the codes seem to agree well with each other (at least for normal incidence) and agree well with experimental observations (although experiments are hard to do with incident energy much less than 1 keV).

In addition to approximations concerning the interactions within the substrate, there are several caveats concerning the nature of the surface:

(1) The computer codes assume an idealized smooth surface down to lattice spacing in MARLOWE and down to interatomic spacing in TRIM. Dr. S. Cohen (PPPL) suggests that machined surfaces will have $\pm 30^\circ$ angle roughness on the 1 micron scale in addition to larger structural irregularities (bellows, etc.). Under some conditions, erosion can lead to dendrites (Eckstein and Verbeek, IPP 9/32 1979, P. 42, for example) or a spongy surface. It is probably easier to make the surface arbitrarily rough (by using, for example, a honeycomb structure

than to make and keep the surface smooth down to lattice spacing. The codes are not set up to consider rough surfaces at this time. However, it may make sense to take the smooth surface results and generate pseudo-rough surface results by averaging the results over a spread of incident angles.

(2) Surface contamination is not included as an option in the codes at this time, although it has been observed to affect the energy spectrum in experiments (e.g. Eckstein and Verbeek, IPP 9/32, 1979, P. 63).

(3) Absorbed interstitial hydrogen or helium or impurities can be included in MARLOWE although I have not yet exercised this option.

Data Tabulation and Transfer

For each type of incident particle and substrate composition, the scattering distribution is a five-dimensional function in terms of the incident energy E, the incident angle α relative to the normal, the outgoing velocity magnitude V, polar angle θ, and azimuthal angle ϕ relative to the plane of the incoming particle and normal, as shown below

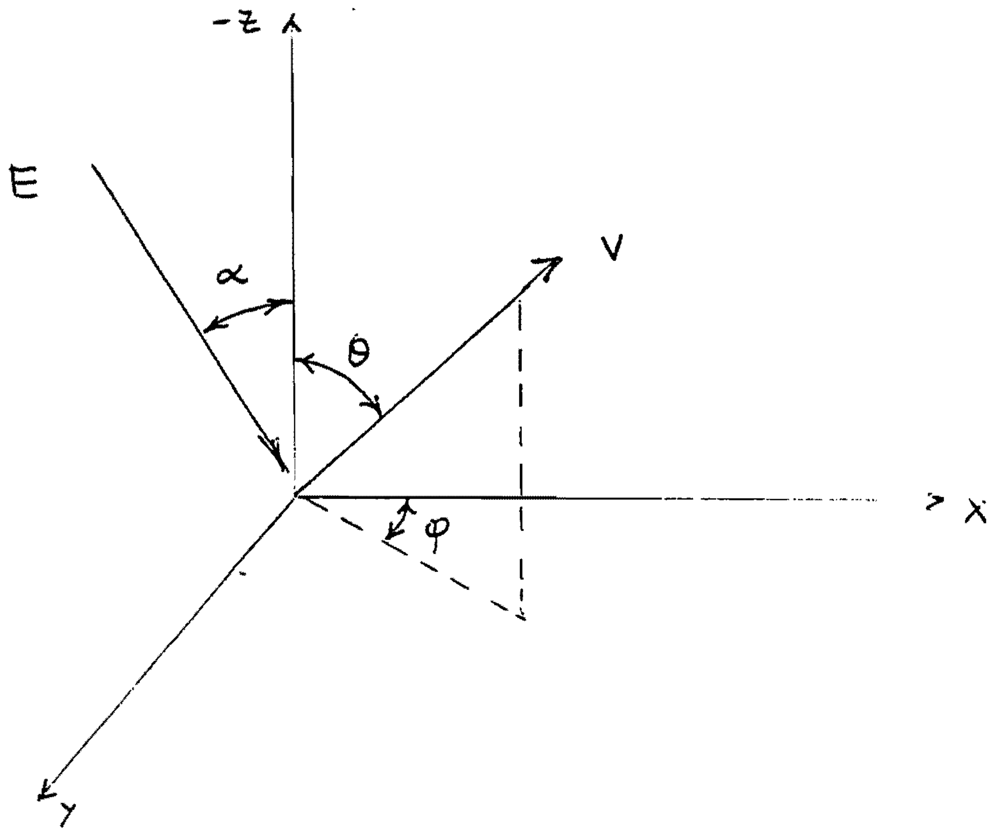

Fig. 1.

Since the distribution is five-dimensional, it was decided that it should be represented (tabulated) by no more than five parameters in each dimension (5^5 = 3125 numbers). Since there are sharp cutoffs in the outgoing velocity spectrum, it was decided to represent the results in spherical coordinates (Fig. 1) even though the results are needed for the Cartesian components of velocity.

Originally it was planned to store the results in the form of the differential distribution function

$$p(v,\theta,\phi;\ E,\alpha)\quad v^2 dv\ \sin\theta\ d\theta\ d\phi.$$

However, the differential distribution can be highly peaked, particularly at grazing incidence, and it would have to be integrated and inverted each time it was used in subsequent Monte Carlo codes. Consequently, a better way of representing and storing the data was developed, based on the inverse cumulative distribition function to be described below.

Cumulative Distribition - 1-D Example

Consider a collection of data points X_I for I = 1, ITOT. Sort these points in, for example, ascending order of X_I. Identify

$$\xi \equiv (I-1)/(ITOT-1)$$

and fit the curve $x = X(\xi)$ for $0 \le \xi \le 1$ to the ordered data points. Then the distribution of the original data points can be reproduced at will by evaluating $x = X(\xi)$ with random variate ξ uniformly distributed in [0,1].

This prescription is the same as setting $x = P^{-1}(\xi)$ = the inverse of the cumulative distribution where

$$P(x) \equiv \int_0^x dx\ p(x)$$

and $p(x)\ dx$ = the probability of finding data points between x and $x + dx$.

Cumulative Distribution - 2-D Example

Consider a collection of data points in two dimensions $(x_I,\ y_I)$ for I = 1, ITOT. Sort on x_I to find $x = X(\xi)$, keeping pairs $(x_I,\ y_I)$

together. Then for any interval $I_1 \leq I \leq I_2$ where $I_2 - I_1 << ITOT$, sort on y_I and let

$$\eta = (I - I_1)/(I_2 - I_1) \qquad 0 \leq \eta \leq 1$$

Fit the curve

$$y = Y(\eta,\xi) \qquad \text{where} \quad \xi \approx \frac{1}{2}(I_1 + I_2)$$

to the data points y_I. This represents an inverse cumulative probability for finding y given ξ in the differential interval

$$(I_1 - 1)/(ITOT - 1) \leq \xi \leq (I_2 - 1)/(ITOT - 1).$$

It is unfortunate that the distribution must be differential in the other dimensions. If we start with 10,000 data points and divide the interval in each dimension into ten subintervals we are left with only ten data points in each subinterval. Nevertheless, by sorting the data into subintervals each containing the same number of data points we make more effective use of the data than if we had sorted into prescribed subintervals in x, y, z to find the differential distribution.

In summary then, the results from the MARLOWE code for scattered atoms are tabulated in the form

$$v = F_1(\xi;\ E,\alpha) \qquad E = \text{incident energy}$$

$$\cos\theta = F_2(\eta,\xi;\ E,\alpha) \qquad \alpha = \text{incident angle}$$

$$\cos\phi = F_3(\zeta,\eta,\xi;\ E,\alpha)$$

from which we can compute the Cartesian components

$$v_x = v \sin\theta \cos\phi$$

$$v_y = \pm v \sin\theta \sin\phi \qquad \text{given left-right symmetry}$$

$$\underline{v}_z = v \cos\theta$$

along the -z axis pointing out of the surface

The function F_1, F_2, and F_3 are tabulated

for $\left\{\begin{matrix}\xi \\ \eta \\ \zeta\end{matrix}\right\} = 0.1, 0.3, 0.5, 0.7, 0.9$

and for $\alpha = 0^\circ, 20^\circ, 40^\circ, 60^\circ, 80^\circ$

$E = 50$ eV, 100 eV, 200 eV, 500 eV, 1000 eV

An example of the namelist input to MARLOWE and the tabulated values of v, $\cos\theta$, and $\cos\phi$ from file XDSS is given on the next two pages. v is given in units of $\sqrt{e.v/AMU}$.

50 eV D → SS 80°

M50D80, BATEMAN, 8 JL 80. DEUTERIUM INCIDENT ON STAINLESS STEEL TARGET.

5.00000E+01 = KINETIC ENERGY OF INCIDENT PARTICLE
8.00000E+01 = POLAR ANGLE FROM NORMAL OF INCIDENT PARTICLE
9.86900E-01 = FRACTION OF INCIDENT PARTICLES REFLECTED
2.01400E+00 = MASS OF INCIDENT PARTICLES IN AMU (INPUT IN DIAG1)

MAGNITUDE OF VELOCITY OF SCATTERED PARTICLES (SI ACROSS)

6.54686E+00	6.70313E+00	6.76220E+00	6.81150E+00	6.87134E+00

COS POLAR ANGLE FROM NORMAL (ETA ACROSS, SI DOWN)

1.25909E-01	3.42020E-01	5.45156E-01	7.35030E-01	9.28397E-01
1.26095E-01	2.74845E-01	4.11108E-01	5.63580E-01	7.65372E-01
1.31922E-01	2.51891E-01	3.58945E-01	4.83603E-01	6.47232E-01
1.12655E-01	2.16707E-01	3.02086E-01	3.99244E-01	5.49632E-01
9.54300E-02	1.73111E-01	2.39628E-01	3.15742E-01	4.28309E-01

COS AZIMUTHAL ANGLE (ZETA ACROSS, ETA DOWN, SI DOWN)

5.76603E-01	9.67811E-01	9.91303E-01	9.97367E-01	9.99734E-01
-2.27908E-01	2.06963E-01	5.33186E-01	8.51474E-01	9.89304E-01
-3.87930E-01	-5.26488E-02	2.54455E-01	6.17360E-01	9.61547E-01
-4.36076E-01	-1.13961E-01	1.56257E-01	5.50565E-01	9.38179E-01
-4.96076E-01	-1.31862E-01	2.08363E-01	5.84495E-01	9.51994E-01
9.17601E-01	9.73207E-01	9.89674E-01	9.97054E-01	9.99629E-01
7.38135E-01	9.08307E-01	9.65724E-01	9.89867E-01	9.98983E-01
6.58308E-01	8.42555E-01	9.36738E-01	9.80575E-01	9.98631E-01
6.21208E-01	8.06302E-01	9.28411E-01	9.72033E-01	9.97037E-01
6.58866E-01	8.15428E-01	9.08394E-01	9.66505E-01	9.97502E-01
9.43432E-01	9.81641E-01	9.92320E-01	9.97752E-01	9.99741E-01
8.64632E-01	9.48390E-01	9.81931E-01	9.93753E-01	9.99171E-01
8.09261E-01	9.22544E-01	9.63581E-01	9.80901E-01	9.98890E-01
7.94511E-01	8.99790E-01	9.54891E-01	9.85192E-01	9.97756E-01

8.16937E-01	9.10344E-01	9.57698E-01	9.86181E-01	9.98763E-01
9.67190E-01	9.85765E-01	9.94486E-01	9.98008E-01	9.99704E-01
9.36279E-01	9.71302E-01	9.88305E-01	9.95254E-01	9.99612E-01
9.13480E-01	9.60403E-01	9.82417E-01	9.93932E-01	9.99446E-01
8.90793E-01	9.49218E-01	9.79412E-01	9.92449E-01	9.99218E-01
9.07674E-01	9.51836E-01	9.78251E-01	9.92930E-01	9.99254E-01
9.87206E-01	9.94237E-01	9.97496E-01	9.99106E-01	9.99931E-01
9.70465E-01	9.86239E-01	9.93594E-01	9.97933E-01	9.99735E-01
9.62314E-01	9.85476E-01	9.92711E-01	9.97397E-01	9.99725E-01
9.50524E-01	9.82999E-01	9.91960E-01	9.96709E-01	9.99547E-01
9.61372E-01	9.82322E-01	9.92161E-01	9.97543E-01	9.99775E-01

```
DISTRIBUTION OF SCATTERED NEUTRALS FROM THE MARLOWE CODE BY M. ROBINSON
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MARLOWE Data set

```
M50D00, BATEMAN, 11 JL 80,  DEUTERIUM INCIDENT ON STAINLESS STEEL TARGET.
 $XTAL ALAT=3*3.615,NTYPE=2,TYPE=2HSS,2HD ,NEIGH=18,0,Z=26.0,1.0,
      W=55.847,2.014,SURFCE=.T.,.F.,INEL=.T.,.T.,.T.,.T. $END
  1     0.5        0.5        0.0     1    0.5       -0.5        0.0    FCC 0010
  1    -0.5        0.5        0.0     1   -0.5       -0.5        0.0    FCC 0020
  1     0.5        0.0        0.5     1    0.5        0.0       -0.5    FCC 0030
  1    -0.5        0.0        0.5     1   -0.5        0.0       -0.5    FCC 0040
  1     0.0        0.5        0.5     1    0.0        0.5       -0.5    FCC 0050
  1     0.0       -0.5        0.5     1    0.0       -0.5       -0.5    FCC 0060
  1     1.0        0.0        0.0     1   -1.0        0.0        0.0    FCC 0070
  1     0.0        1.0        0.0     1    0.0       -1.0        0.0    FCC 0080
  1     0.0        0.0        1.0     1    0.0        0.0       -1.0    FCC 0090
 $SURF RSORT=0.,0.,1.,AXISA=1.,0.,0.,AXISB=0.,1.,0.,SIDEA=1.,SIDEB=1.,
CALC=.T.,.T. $END
 $MODL RB=0.42,0.42,EDISP=10.,0.,EQUIT=9.5,5.0,EBND=0.5,0.0,
      TIM(15)=.F.,POLY=.T.,.T. $END
 $OUTP INFORM=4*.T.,INFORM(6)=.T. $END
 $PROJ LOG=20,LAIF=2,THA=00.0,EKIP=50.,MAXRUN=20000,PRIM=.T.,.T. $END
 $PROJ MAXRUN=-1 $END
```

50 eV D → SS 0°

```
M50D00, BATEMAN, 9 JL 80,  DEUTERIUM INCIDENT ON STAINLESS STEEL TARGET.

  5.00000E+01 = KINETIC ENERGY OF INCIDENT PARTICLE
  0.          = POLAR ANGLE FROM NORMAL OF INCIDENT PARTICLE
  5.33600E-01 = FRACTION OF INCIDENT PARTICLES REFLECTED
  2.01400E+00 = MASS OF INCIDENT PARTICLES IN AMU (INPUT IN DIAG1)

MAGNITUDE OF VELOCITY OF SCATTERED PARTICLES (SI ACROSS)
  4.14796E+00  5.43136E+00  6.01222E+00  6.34972E+00  6.53511E+00

COS POLAR ANGLE FROM NORMAL (ETA ACROSS, SI DOWN)
  5.55615E-01  7.30122E-01  8.33068E-01  9.07914E-01  9.72892E-01
  5.27205E-01  7.13938E-01  8.21469E-01  9.00366E-01  9.70520E-01
  5.05029E-01  6.84957E-01  8.01173E-01  8.85867E-01  9.62672E-01
  4.99026E-01  6.88997E-01  8.06735E-01  8.92685E-01  9.66537E-01
  3.38775E-01  4.79995E-01  5.82141E-01  6.74107E-01  7.90920E-01

COS AZIMUTHAL ANGLE (ZETA ACROSS, ETA DOWN, SI DOWN)
 -9.55600E-01 -5.76667E-01 -6.47741E-03  6.03588E-01  9.49299E-01
 -9.30220E-01 -5.86609E-01 -9.17408E-02  5.01725E-01  9.21081E-01
 -9.33387E-01 -5.37984E-01  1.51195E-02  5.29199E-01  9.18403E-01
 -9.47814E-01 -5.99912E-01 -5.42763E-02  5.10378E-01  9.49255E-01
 -9.40743E-01 -5.11007E-01  1.92819E-01  6.65997E-01  9.47559E-01
 -9.24703E-01 -5.68625E-01 -2.23915E-02  5.79727E-01  9.36458E-01
 -9.54706E-01 -5.76301E-01  4.13930E-02  5.76660E-01  9.53131E-01
 -9.43172E-01 -6.17221E-01 -1.08521E-01  5.11090E-01  9.16170E-01
 -9.24470E-01 -4.99517E-01  8.04717E-02  6.55091E-01  9.63264E-01
 -9.43005E-01 -6.00098E-01 -8.05098E-02  4.96404E-01  9.42011E-01
 -9.39374E-01 -5.96629E-01 -2.06845E-02  5.79261E-01  9.31016E-01
 -9.56049E-01 -6.29250E-01 -6.67243E-02  5.39674E-01  9.14811E-01
 -9.00740E-01 -5.05576E-01  1.95047E-01  6.93110E-01  9.60451E-01
 -9.53605E-01 -5.95527E-01  5.20529E-02  5.89037E-01  9.40754E-01
 -9.29367E-01 -5.75353E-01 -2.20431E-02  5.44215E-01  9.50069E-01
 -9.44005E-01 -5.78528E-01 -4.10664E-02  5.49971E-01  9.51292E-01
 -9.51224E-01 -5.50495E-01 -2.71032E-02  6.06977E-01  9.41420E-01
 -9.10720E-01 -5.51067E-01  2.76381E-02  5.55206E-01  9.55897E-01



 -9.36527E-01 -5.33237E-01  6.90861E-02  6.11501E-01  9.53653E-01
 -9.70330E-01 -6.86663E-01 -1.00030E-01  4.36004E-01  9.35164E-01
 -9.41227E-01 -5.92032E-01 -1.01730E-02  5.77624E-01  9.45891E-01
 -9.43979E-01 -5.46351E-01  7.14162E-02  6.34735E-01  9.59453E-01
 -9.50262E-01 -5.17653E-01 -3.26586E-03  6.39330E-01  9.30000E-01
 -9.50054E-01 -5.94062E-01 -4.72912E-02  5.17105E-01  9.51030E-01
 -9.25116E-01 -6.08899E-01 -1.08300E-01  5.15239E-01  9.53503E-01
```

1 keV D → SS 0°

MIKDOO, BATEMAN, 21 JL 80, DEUTERIUM INCIDENT ON STAINLESS STEEL TARGET.

1.00000E+03	=	KINETIC ENERGY OF INCIDENT PARTICLE
0.	=	POLAR ANGLE FROM NORMAL OF INCIDENT PARTICLE
3.28600E-01	=	FRACTION OF INCIDENT PARTICLES REFLECTED
2.01400E+00	=	MASS OF INCIDENT PARTICLES IN AMU (INPUT IN DIAG1)

MAGNITUDE OF VELOCITY OF SCATTERED PARTICLES (SI ACROSS)

1.45831E+01	2.00691E+01	2.33418E+01	2.58467E+01	2.83984E+01

COS POLAR ANGLE FROM NORMAL (ETA ACROSS, SI DOWN)

4.54189E-01	6.52993E-01	7.70530E-01	8.79424E-01	9.60058E-01
4.52986E-01	6.31678E-01	7.69403E-01	8.63030E-01	9.53408E-01
4.11749E-01	6.16463E-01	7.62599E-01	8.67895E-01	9.59698E-01
3.89640E-01	5.92512E-01	7.50740E-01	8.58292E-01	9.54744E-01
3.22452E-01	5.14785E-01	6.52784E-01	7.80373E-01	9.17193E-01

COS AZIMUTHAL ANGLE (ZETA ACROSS, ETA DOWN, SI DOWN)

-9.07532E-01	-5.62713E-01	2.49705E-02	5.16734E-01	9.89499E-01
-9.70499E-01	-5.84860E-01	8.05242E-02	6.20436E-01	9.42623E-01
-9.57251E-01	-6.02729E-01	-1.29443E-01	5.63226E-01	9.32578E-01
-9.10233E-01	-5.40319E-01	-7.24630E-03	5.64323E-01	9.43780E-01
-9.28076E-01	-5.51735E-01	2.45938E-02	6.23978E-01	9.72196E-01
-9.18133E-01	-6.08062E-01	-8.02676E-02	5.55392E-01	9.45452E-01
-9.83871E-01	-4.95741E-01	5.82079E-02	5.43846E-01	9.61253E-01
-9.07563E-01	-6.66626E-01	-1.69723E-01	5.14374E-01	9.83449E-01
-9.43777E-01	-6.11901E-01	1.07854E-01	5.03117E-01	9.51719E-01
-9.22376E-01	-4.15537E-01	1.79305E-01	6.30130E-01	9.45256E-01
-9.24446E-01	-5.30094E-01	9.08942E-02	6.59421E-01	9.41678E-01
-9.57180E-01	-6.51336E-01	6.69216E-03	5.14542E-01	9.39216E-01
-9.05208E-01	-5.69203E-01	-1.06874E-01	4.37606E-01	9.10348E-01
-9.81056E-01	-4.22000E-01	1.10902E-01	6.14343E-01	9.55930E-01
-9.41436E-01	-6.31725E-01	-5.01630E-02	5.18137E-01	8.82302E-01
-9.36443E-01	-5.84327E-01	-4.89053E-02	5.98401E-01	9.68237E-01
-9.12338E-01	-4.00758E-01	1.16010E-01	6.04253E-01	9.46587E-01
-9.06324E-01	-5.56668E-01	6.07141E-02	6.37703E-01	9.58538E-01
-9.40067E-01	-4.66624E-01	1.04287E-01	6.13544E-01	9.52156E-01
-9.43799E-01	-5.28818E-01	-1.52586E-01	4.07904E-01	9.87264E-01
-9.66540E-01	-6.31349E-01	-8.11897E-02	6.34510E-01	9.67528E-01
-9.26510E-01	-4.39932E-01	2.22905E-02	6.22455E-01	9.33471E-01
-9.00659E-01	-5.02870E-01	7.31059E-02	5.93691E-01	9.73177E-01
-9.10270E-01	-6.14385E-01	9.09833E-02	5.61120E-01	9.46895E-01
-9.42364E-01	-5.61615E-01	-2.70612E-02	5.96051E-01	9.36133E-01

1 keV D → SS 30°

MIKDOO, BATEMAN, 21 JL 80, DEUTERIUM INCIDENT ON STAINLESS STEEL TARGET.

1.00000E+03 = KINETIC ENERGY OF INCIDENT PARTICLE
3.00000E+01 = POLAR ANGLE FROM NORMAL OF INCIDENT PARTICLE
7.01100E-01 = FRACTION OF INCIDENT PARTICLES REFLECTED
2.01400E+00 = MASS OF INCIDENT PARTICLES IN AMU (INPUT IN DIAG1)

MAGNITUDE OF VELOCITY OF SCATTERED PARTICLES (SI ACROSS)

2.29601E+01	2.86461E+01	3.01427E+01	3.06546E+01	3.09064E+01

COS POLAR ANGLE FROM NORMAL (ETA ACROSS, SI DOWN)

3.95005E-01	5.83416E-01	7.23119E-01	8.40658E-01	9.40877E-01

2.40269E-01	3.93982E-01	5.30704E-01	6.83156E-01	8.72329E-01
1.57540E-01	2.44547E-01	3.46329E-01	4.89835E-01	7.46949E-01
9.43558E-02	1.44037E-01	1.99525E-01	2.88999E-01	4.94757E-01
9.71978E-02	1.38971E-01	1.86957E-01	2.50553E-01	3.92800E-01

COS AZIMUTHAL ANGLE (ZETA ACROSS, ETA DOWN, SI DOWN)

-9.33427E-01	-4.91246E-01	1.39483E-01	6.55920E-01	9.53076E-01
-9.49494E-01	-4.80141E-01	1.81302E-01	6.80956E-01	9.61555E-01
-9.27352E-01	-5.18642E-01	1.14265E-01	6.49942E-01	9.66266E-01
-9.51449E-01	-5.39431E-01	1.40168E-01	7.06596E-01	9.51951E-01
-9.36943E-01	-5.83649E-01	1.61282E-02	6.46215E-01	9.71895E-01
-5.93034E-01	3.34125E-01	7.76090E-01	9.14221E-01	9.96344E-01
-4.70595E-01	4.14444E-01	7.55273E-01	9.28750E-01	9.92035E-01
-4.03435E-01	2.50459E-01	6.77063E-01	9.05634E-01	9.91029E-01
-7.51900E-01	3.62832E-02	5.18645E-01	8.44572E-01	9.79824E-01
-9.11037E-01	-2.95082E-01	3.40327E-01	8.07312E-01	9.73958E-01
5.22750E-01	8.51936E-01	9.50282E-01	9.83099E-01	9.98124E-01
5.79019E-01	8.88722E-01	9.59917E-01	9.88000E-01	9.98742E-01
4.59251E-01	8.26069E-01	9.38363E-01	9.83106E-01	9.98256E-01
3.11593E-01	7.14722E-01	8.71690E-01	9.64765E-01	9.91329E-01
1.57306E-01	5.19890E-01	7.78431E-01	9.16356E-01	9.86764E-01
9.27784E-01	9.84291E-01	9.93882E-01	9.98443E-01	9.99775E-01
9.03719E-01	9.73516E-01	9.89124E-01	9.96396E-01	9.99705E-01
8.40984E-01	9.52625E-01	9.80867E-01	9.94081E-01	9.99360E-01
7.88739E-01	9.19189E-01	9.70085E-01	9.89615E-01	9.98048E-01
7.55931E-01	8.77313E-01	9.48810E-01	9.82632E-01	9.97765E-01
9.74799E-01	9.91481E-01	9.96838E-01	9.98911E-01	9.99932E-01
9.62241E-01	9.86138E-01	9.95071E-01	9.98717E-01	9.99817E-01
9.35949E-01	9.76109E-01	9.98800E-01	9.96696E-01	9.99637E-01
9.16670E-01	9.65201E-01	9.87706E-01	9.95410E-01	9.99410E-01
9.13539E-01	9.61965E-01	9.83939E-01	9.94693E-01	9.99090E-01

Results

For deuterium scattering off stainless steel (amorphous model with a smooth surface) the reflection coefficient R_N (= the number of particles scattered back through the front surface divided by the total number of incident particles) varies more strongly with incident angle α than with incident energy, as shown in Fig. 2. At normal incidence ($\alpha = 0^\circ$) the reflection coefficient agrees with other published computations and with experimental observations to within 10% as tabulated below (from Eckstein and Verbeek, IPP 9/32, 1979)

$D \rightarrow SS \quad \alpha = 0^\circ$

E	R_N from present study	R_N other computation	R_N experimental
50 eV	.5333	.53	--
100	.486	.47	.52
200	.432	.43	.45
500	.373	.40	.40
1 keV	.329	.35	.31

At grazing incidence, almost all the particles are reflected, even at high energy.

At normal incidence, the reflected velocity spectrum is broad, with most of the scattered particles retaining between 50% and 90% of their incident velocity. The spectrum shifts downward with increasing incident energy as shown in Fig. 3. At grazing incidence (e.g. $\alpha = 80^\circ$) most of the scattered particles retain more than 90% of their incident velocity, since the particles generally spend less time in the substrate.

In some of the runs, the distribution of the polar angle was analyzed without regard to scattered energy or azimuthal angle, $\cos\theta = P^{-1}(\xi;\ E,\alpha)$ as shown in Figs. 4 and 5. At normal incidence, if the differential distribution followed the usually expected $\cos\theta$ dependence, then

$$\xi = P(\theta) = 2\int_0^\theta d\theta \sin\theta \cos\theta = \cos^2\theta \ .$$

However, instead of observing $\cos\theta = \xi^{1/2}$, we observed $\cos\theta = \xi^{0.37}$ for 100 eV incidence and intermediate behavior for 1 keV incidence. This observation of preferential backscattering is consistent with data from TRIM (from Haggmark, 1980) and with published data (O.S. Oen and M.T. Robinson, Nucl. Inst. and Math., 132, 1976, P. 651, Fig. 5d).

At grazing incidence, there seems to be a discrepancy between the MARLOWE and TRIM codes (for $D \rightarrow SS$, $E = 100$ eV, $\alpha = 80^\circ$) as shown in Fig. 5. The TRIM code indicates a distribution that is much more tightly peaked around the specular reflection angle. One possible reason for the discrepancy may be that the surface is effectively more rough in the MARLOWE code, with atoms typically spaced a lattice distance apart (3.615 Å here) in the MARLOWE code and spaced the nearest neighbor distance apart (2.5 Å) in the TRIM code. Differences in the way angular scattering is computed in the two codes may also be responsible.

As the data is normally processed, the spread in polar angle depends upon the scattered energy and the spread in the azimuthal angle depends upon both the scattered energy and polar angle. Plotted as a function of incident angle α, Fig. 6 shows the spread in scattered polar angles for particles in the middle of the scattered energy spectrum $\xi = .5$ and Fig. 7 shows the spread in scattered azimuthal angles for particles in the middle of both the scattered energy spectrum $\xi = .5$ and polar angle spectrum $\eta = .5$, for 50 eV incident deuterous. It can be seen that the spread in azimuthal angle is comparable to the spread in poloidal angle for particles with grazing incidence. The non-monotonic curves in the plot of azimuthal angles, indicating some bunching of scattered particles away from the forward angle, seems to be qualitatively consistent with recent computational and experimental observations by W. Eckstein and H. Verbeek (4th Intern. Conf. on Plasma Surface Interactions, Garmisch-Partenkirchen, 1980).

Acknowledgements

This research was carried out at the request of Dr. Douglass E. Post. Many helpful suggestions were offered by Drs. David Larrabee, Daniel Heifetz, Allen Boozer, Mark Robinson, Lee Haggmark, Sam Cohen, John Kinney, and by members of the Tokamak Modeling Group.

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REFERENCES

(1) W. Eckstein and H. Verbeek, IPP 9/32 (Aug. 1979), Data on light ion reflection, 83 pages, Massive compendium of results both computational and experimental.

(2) G. M. McCracken and P. E. Stott, Nuclear Fusion 19, 889-981, (1979), Plasma - Surface Interactions in Tokamaks.

(3) Rainer Behrisch, Erice Summer School 1976 of Tokamak Results for Breakeven Plasma-Wall Interactions.

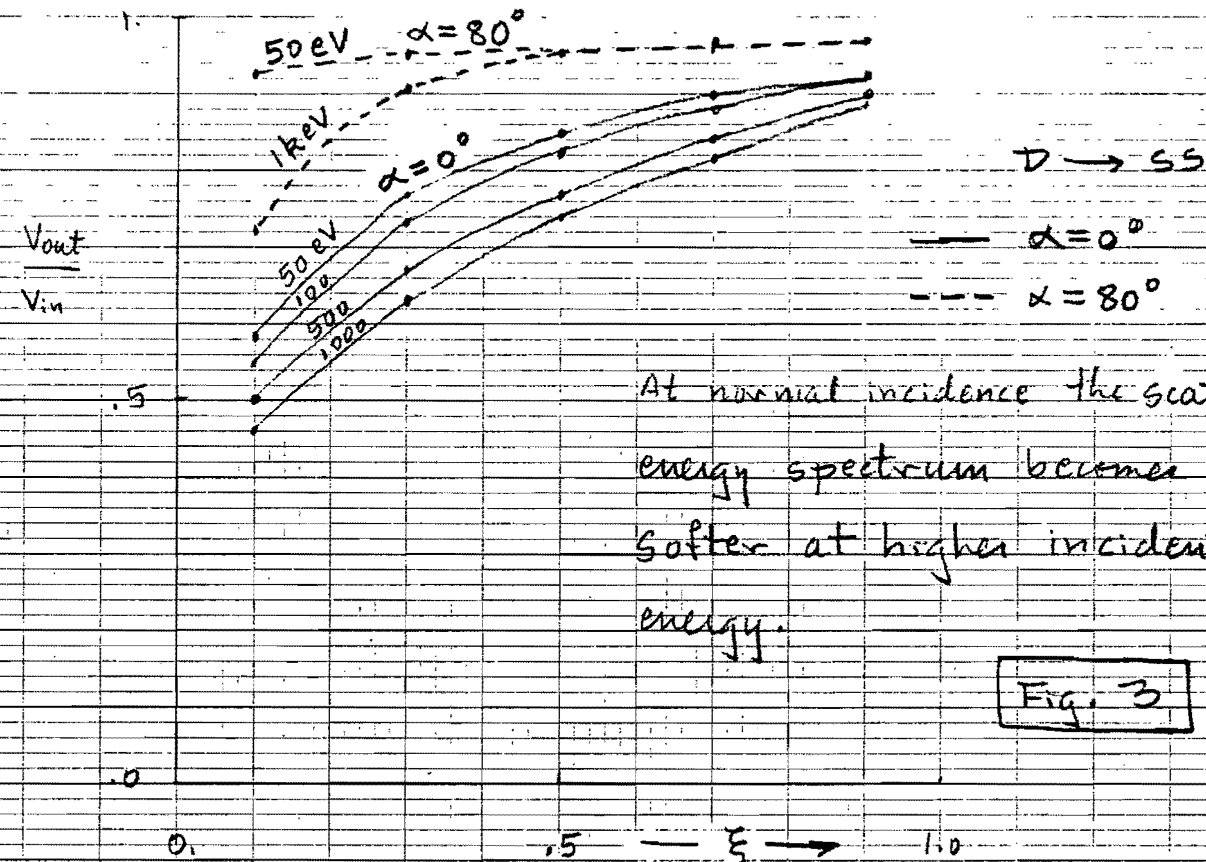
(4) W. Eckstein, H. Verbeek, and J. P. Biersack, J. Appl. Phys. 51, 1194-1200, (1980), Comparison between MARLOWE and TRIM computer code results.

(5) H. Berbeek, W. Eckstein, and R. S. Bhattacharya, J. Appl. Phys. 51, 1783-1789, (1980), Comparison between TRIM computed results and scattering experiments.

(6) Mark Robinson, 8, 624, 5791 MARLOWE.

(7) Lee Haggmark, 8, 532, 3148 TRIM.

23 July 1980



At normal incidence the scattered energy spectrum becomes softer at higher incident energy.

Fig. 3

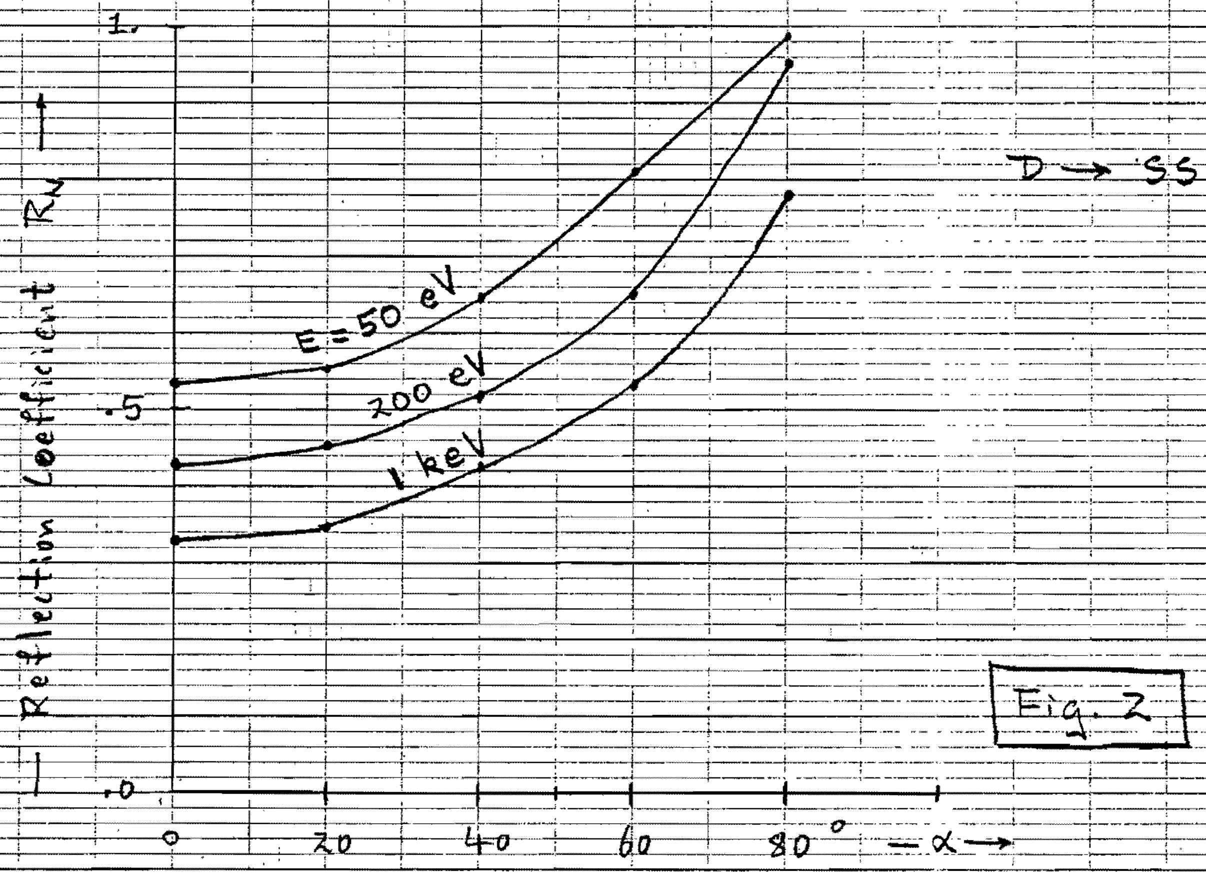


Fig. 2

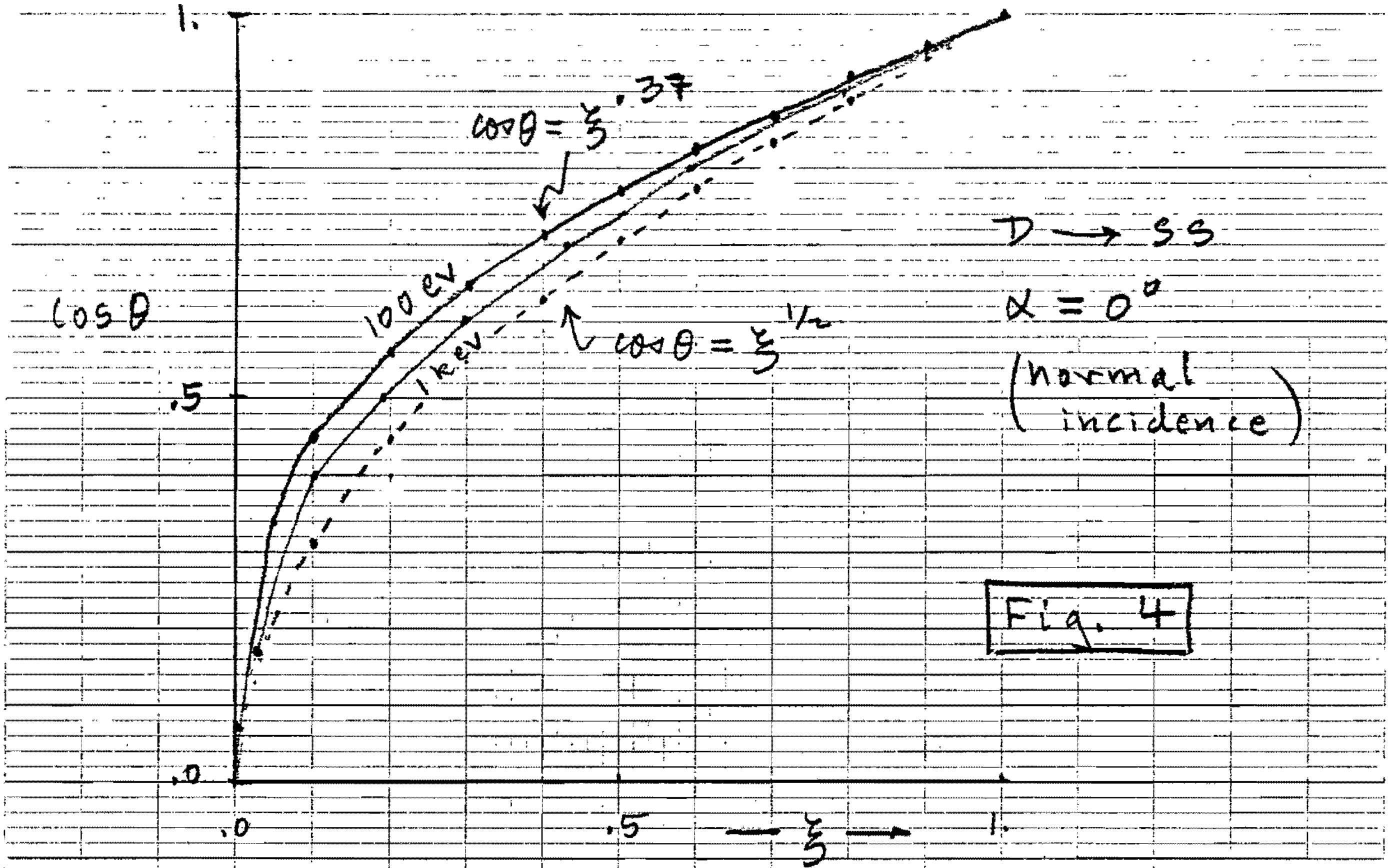

1.
cos θ = ξ^.37
100 eV
1 keV
cos θ = ξ^1/2
cos θ
.5
.0
.5
— ξ —→
1.
D → SS
α = 0°
(normal incidence)

Fig. 4

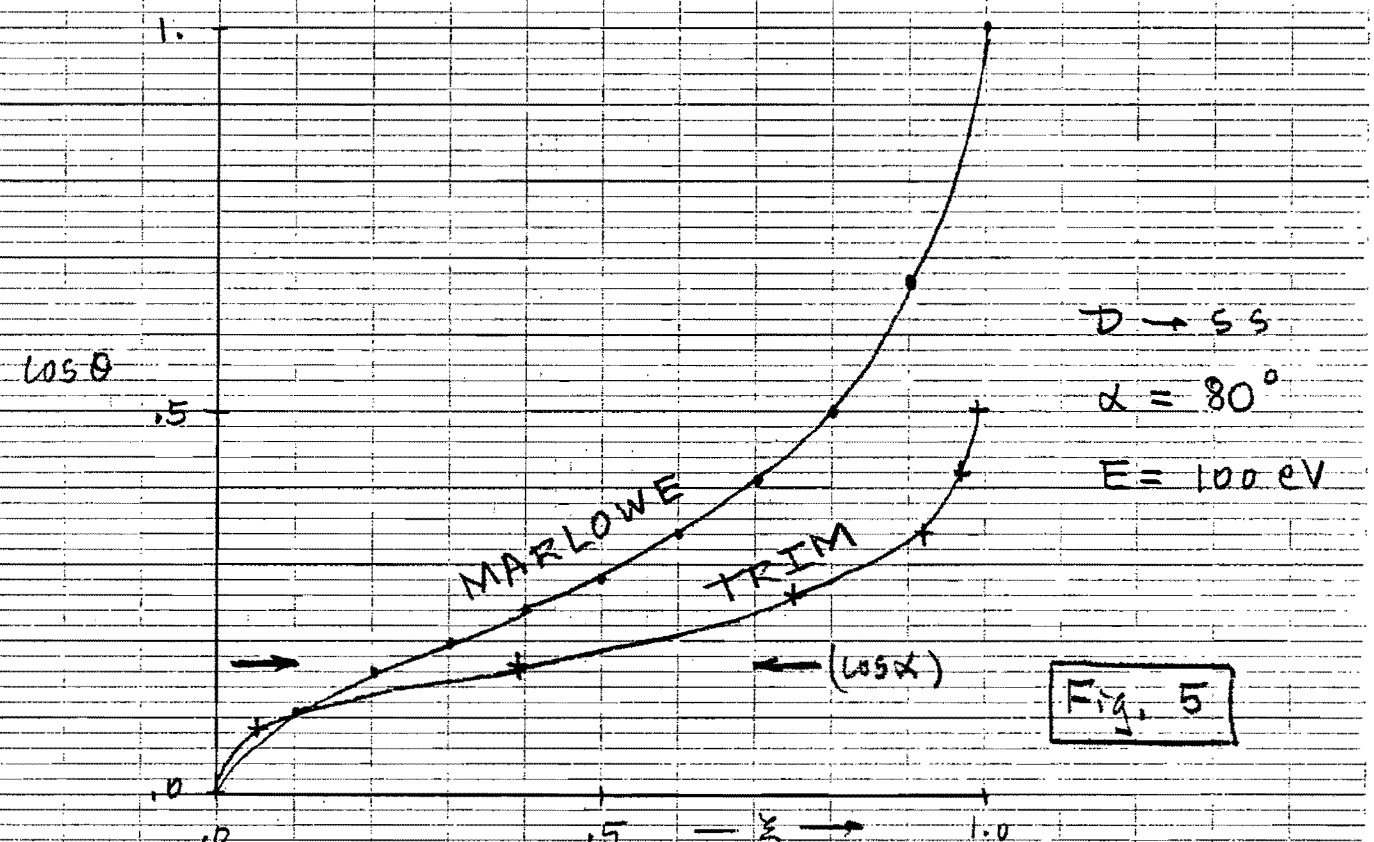

1.
cos θ
.5
.0
.0
.5
— ξ —→
1.0
MARLOWE
TRIM
←(cos α)
D → SS
α = 80°
E = 100 eV

Fig. 5

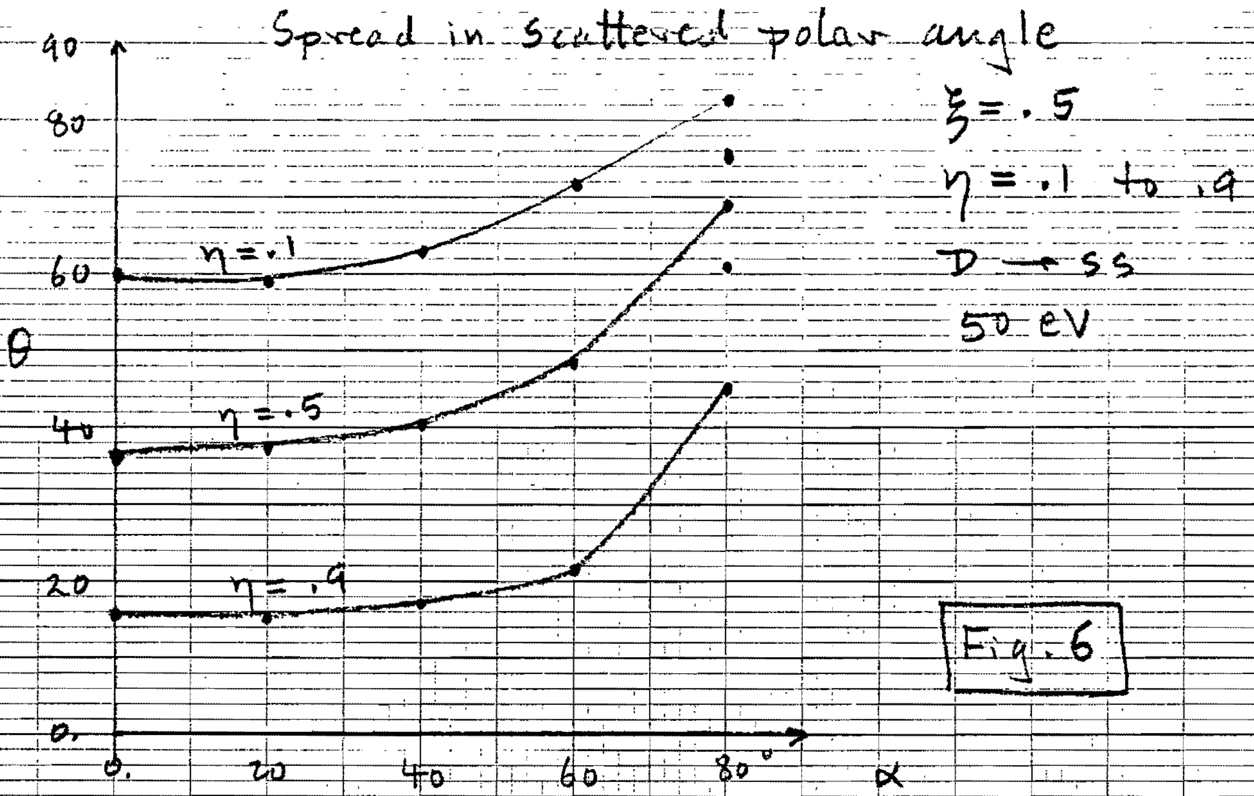

Spread in scattered polar angle
θ
90
80
60
40
20
0.
0.
20
40
60
80°
α
η = .1
η = .5
η = .9
ξ = .5
η = .1 to .9
D → SS
50 eV

Fig. 6

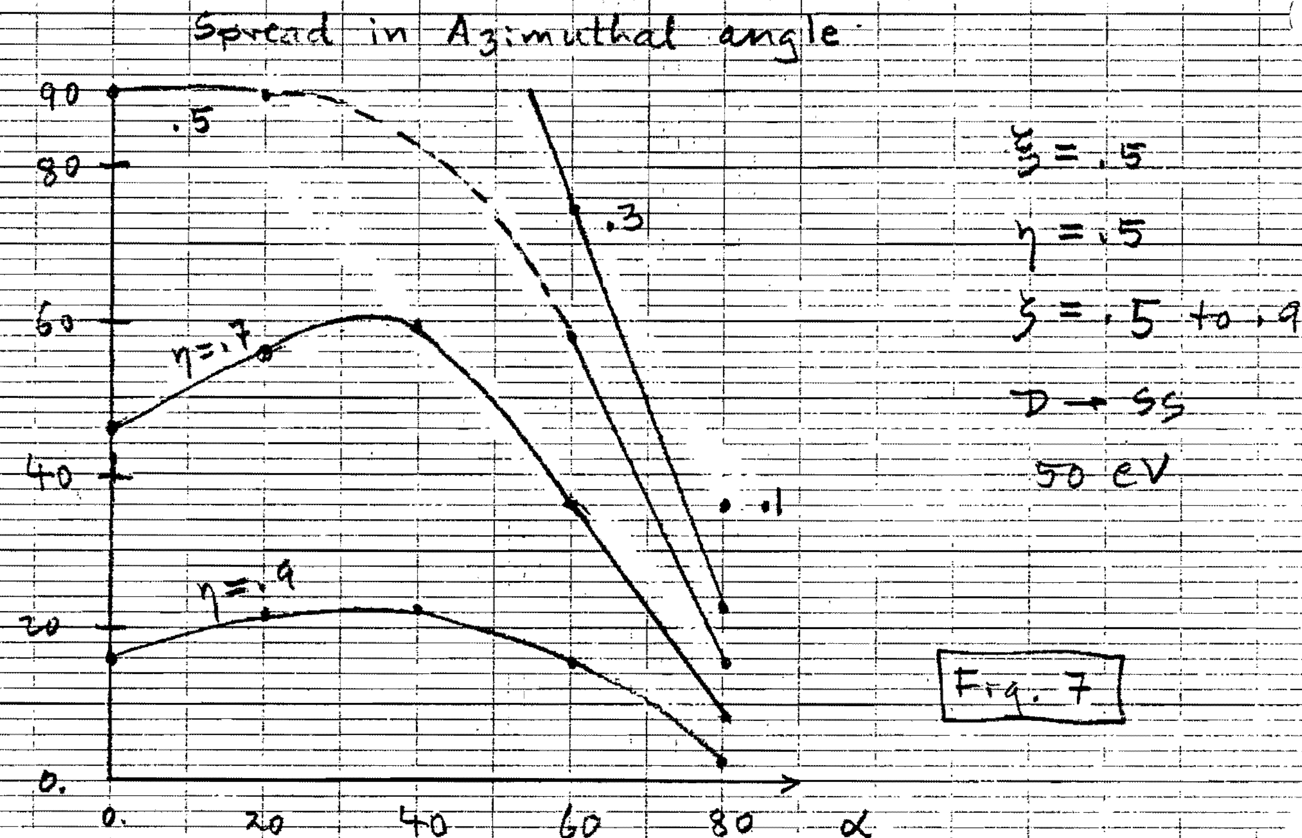

Spread in Azimuthal angle
φ
90
80
60
40
20
0.
0.
20
40
60
80
α
.5
.3
.1
η = .7
η = .9
ξ = .5
η = .5
ξ = .5 to .9
D → SS
50 eV

Fig. 7

How to compile and run the MARLOWE and diagnostic codes

My copies of the sourch decks for MARLOWE and diagnostic codes can be obtained on the MFE 7600 computer by typing

FILEM - READ - 4270 - .MARLOWE - MARLGB1 - DIAG1 -...

where

MARLGB1 = MARLOWE source deck with unformatted output of the scattered velocities

RMI = controllee made from MARLGB1

SUBM = Cosmos file to run RM1 includes input data

INPUT = separate input data file

DIAG1 = source deck for diagnostic code

RD1 = controllee made from DIAG1

SUBD = Cosmos file to run RD1 and construct XDSS

Output files are stored in

FILEM READ 4270 .MARLOWE XDSS ...

where

XDSS = final tabulated results for D → SS

T = unformatted output from each MARLOWE run

M = formatted output from each MARLOWE run

S = typical submit (cosmos) files for MARLOWE

To compile and run a program using LASLFTN type

```
LIX  LASLFTN   SKIPSUM
GETR*  FTN FTNLIB  FTNLIB1  FTNLMAK
GETR*  SLOPE2  SYS2  COMPACT
           FTNMTH1  FTNMTH2  FTNMTH3
           LODF
END
```

To compile a small code such as DIAG1, type

FTN - (I = source, CNAME = controllee, GO) / t v

given a source file, this produces a controllee and runs code

the controllee can be used over again by typing

controllee / t v)

To compile the <u>MARLOWE</u> code, type

```
FTN - (I = source, OPT = 2, LCM = I,
           RFLS = 150000B, RFLL = 500000B,
           GLIB = /*MATH, (Name = controllee) / t  v
```

<u>Helpful people</u>

Mark Robinson (ORNL) 8 624 5791

wrote the MARLOWE code and has provided a lot of useful information.

John Kinney (LLL) 8 532 6669

runs version of MARLOWE code on the MFE 7600 sources file FORSCAT to be compiles using LASLFTN.

Carol Tull (LLL) 8 532 1556

knows how to use LASLFTN

Hoffney Atoya (U. Wisc.) 608-263-4692

8 262 1234 ask for 3-4692

may have version of MARLOWE on the CRAY.

Lee Haggmark (Sandia, Livermore) 8 532 3148

responsible for the TRIM computer code.