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Report



A MONTE-CARLO COMPUTER PROGRAM FOR  
ANALYSIS OF BACKSCATTERING AND SPUTTERING  
IN PRACTICAL VACUUM SYSTEMS

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# A MONTE-CARLO COMPUTER PROGRAM FOR ANALYSIS OF BACKSCATTERING AND SPUTTERING IN PRACTICAL VACUUM SYSTEMS\*

K P Brown

## A B S T R A C T

A Monte Carlo computer program originally developed for analysis of molecular gas flow in axi-symmetric vacuum systems has been extended to include modelling of high energy backscattering and sputtering processes. This report describes the input data required by the computer program together with the results produced. A general description is given of the program operation and the backscattering and sputtering modelling used. An example calculation is included to illustrate practical application of the program.

\*The Monte-Carlo computer program described in this report was developed under joint JET and Culham sponsorship.

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## 1. INTRODUCTION

1.1 The Monte Carlo computer program for studying free molecular gas flow in vacuum structures developed at Culham by J N Chubb<sup>(1,2)</sup> has been extended under joint JET and Culham sponsorship to include modelling of high energy backscattering and sputtering processes.

1.2 The objective in developing this program has been to provide a tool which can be used to investigate and model back-scattering, sputtering and free molecular gas flow in practical situations with a minimum understanding of computer technology.

1.3 The aim of this report is to describe the input data required by the Monte Carlo computer program, the method of running the program on the ICL 4/70 computer at Culham and the output presentation of results. Examples of some studies using the computer program are given in a companion report<sup>(3)</sup>.

## 2. DESCRIPTION OF PROGRAM OPERATION

2.1 An outline flowchart showing the basic program operation is given in Appendix I. A general description of the program operation and the backscattering and sputtering techniques is given in Appendix II.

## 3. RUNNING THE PROGRAM

3.1 The Monte Carlo computer program runs on the ICL 4/70 computer at Culham. To run this program, the user must set up the data file containing the structure parameters described in section 5, and a procedure file containing the necessary job control statements for submitting the program to the job queue. To assist the user in running this program, an example run is given in Appendix III which relates to a "pocket" structure shown in Figure 5. The example shows the setting up of the data and procedure files and the submission of the program to the job queue. The results output by the program for this example run are given in Appendix IV.

## 4. INPUT DATA PRESENTATION

4.1 The input data required by the Monte Carlo computer program can be considered in three sections. The first of these describes the species and energy of primary particles, the number to be studied and the method of their introduction to the structure. The second section describes the presentation of the structure as a series of co-axial cones and cylinders, and section three describes the data required to define the substrate materials used in the structure, together with sputtering and adsorption coefficients for each element of the structure.

### 5. INPUT DATA FORMATS

5.1 Section one of the input data requires three (optionally four) data cards. The first of these cards defines the following parameters in (3I7, 3F14.7, 7X, I2) format:

ICASE IREF INCOME RINNR ROUTR RCENTR  
INAXIS

The meaning of these parameters is described in Table 1.

5.2 The second data card is optional and must be specified only when INAXIS = 3. This card defines the following parameters in (3D12.5) format:

TAL TAM TAN

The purpose of these parameters is explained in Table 2.

5.3 The next data card in this section defines the number and type of primary particles to be studied using the following parameters in (2I7, F12.3, I4, F12.3) format

NP IPRINT ENERGY IZ1 AM1

The meaning of these parameters is described in Table 3.

5.4 The last card in section one of the input data defines the following parameters

in (3I7) format:

NCS NADS NSUB

The meaning of these parameters is given in Table 4.

5.5 Section two of the input data describes the structure as a series of co-axial cones and cylinders. The general form of the structure handled by the program is illustrated in Figure 1. Each length element of the structure is defined by the radii of the inner and outer surfaces at each end of the element and by the element length. Since the output-side radii of one element are the input-side radii of the next element, each element may be specified using only the input-side radii and the element length. The output-side radii of the last element must however be specified. Diaphragms can be simulated by defining zero length conical elements. It should be noted that due to the methods used by the program, all nominally zero length elements must be treated as of some finite value. The length is calculated as  $2 \times 10^{-3} \times$  the radial difference between the input and output ends of the length element. Since inner and outer elements are used, the length is derived from the maximum of the two radial differences.

5.6 Each length element of the structure is specified on a single data card by the following parameters in (3F14.7,7I3) format:

RI RO A MREF IADSOII IADSOI IADSAO  
ISUBII ISUBOI ISUBAO

The meaning of these parameters is given in Table 5.

5.7 Section three of the input data contains the adsorption and substrate details indexed in section two (see Table 5). The next NADS data cards define the adsorption details for the different surfaces used in the structure, each card defining the following parameters in (I3,F8.5,F12.3) format:

IADS ADS1 THR1

The meaning of the parameters is given in Table 6.

5.8 Since backscattering and sputtering processes depend upon both incident particle species and substrate material, it is necessary to define the substrate materials in terms of both species. The next NSUB cards define each substrate material used in the structure using the following parameters in (3I4, 2F8.3,F6.2, 2F12.3,D12.4,F7.4) format:

ISUB IZA1 IZA2 AMASS ADEN RNGE RNEN  
STH EMP1 EMP2

The meaning of these parameters is given in Table 7.

5.9 The user may find it useful to note that more adsorption or substrate material details may be provided than are used in the structure. This allows a standard set of these cards to be included with each different structure with the program indexing only the required details within the structure defined in section 5.6.

5.10 When graphical output is required (ICASE > 999) a further data card is required. This card can contain any alphanumeric data up to a maximum of 60 characters, and could for example give a title for the structure being studied.

5.11 It is possible to submit data for several different structures during one run of the program. To terminate the data, the user must supply a single initial data card with ICASE < 0 at the end of the card deck as shown in the example given in Figure 6.

## 6. TIMING

6.1 Since structures vary a great deal in complexity, it is difficult to give much guidance on the amount of time the program will take to run. For the calculations performed for JET<sup>(3)</sup>, the average time per particle history varied from around 0.1 seconds to 0.5 seconds. In the example given in Appendix III, a total of around 15 minutes computer time was required to study 2000 particles. To

assist the user, the program outputs the average time per particle history. Since this value will be almost constant for a particular structure, it is possible to estimate the amount of time required for further calculations using a similar structure.

6.2 On the ICL 4/70, computer time is allocated to a job in ETU's (elapsed time units) and 1 hour's central processor time is equivalent to 1000 ETU's. The allocation of ETU's to a job is specified by the time parameter on the "SCHEDULE" card of the procedure file. In the example procedure file given in Figure 7, a time allocation of 250 ETU's has been specified representing around 15 minutes' processing time.

6.3 If insufficient time is allocated to a run of the program, results are output for all particle histories studied within the time available.

6.4 At Culham, computer costs vary with the time of day a program is run. Users are advised to run the Monte Carlo program during the overnight period, since charges for program store and time units are least during this period.

## 7. RESULTS OUTPUT BY THE PROGRAM

7.1 A typical set of results output by the Monte Carlo program is given in Appendix IV. These results relate to the JET "pocket" calculation described in Appendix III and are printed out in eight sections. The first section of the printout gives a listing of the structure details, together with information about the primary particle species and its method of introduction to the structure.

7.2 Section two of the printout has been included for diagnostic purposes and shows the tables of direction cosines for angles of deflection used in the "multiple scattering model." This section can be ignored by the general user.

7.3 The third section gives the total numbers of primary and sputtered particles adsorbed in the structure, transmitted through the output-end orifice, and

reflected back through the input-end orifice. In the example of the JET "pocket" calculation, the structure was closed at both ends so that all particles introduced were eventually adsorbed. The dispersion, probability and percentage error factors relate to the statistics of adsorption, transmission or reflection events.

7.4 Section four (identified as "Table 1") gives the distribution along the structure of the adsorptions and interactions of primary and sputtered particles for the inner and outer elements. Also included in this table is the distribution of generated sputtered particles. Element numbers and adsorption and substrate index numbers are included to aid correlation of results with the form of the structure described in section one of the printout. The "Adsorptions," "Interactions" and "Generated" columns give the total numbers of those events which have occurred on each surface of each element for the total number of particle histories studied up to the time of printout. For each element three lines of output are printed. The first line refers to events on the inside surface of the inner element, the second line refers to events on the outside surface of the inner element, and the third line refers to the inside surface of the outer element.

7.5 The fifth section of printout ("Table 2") gives the distribution along the structure of the interactions and interaction probabilities per unit area of the primary and sputtered particles for the inner and outer elements. As in "Table 1," the element numbers are included and the output for each element appears on three lines referring to the inside of the inner element, the outside of the inner element, and the inside of the outer element respectively. The interactions column gives the total numbers of interactions on each surface of each element for the total number of particles studied up to the time of printout.

7.6 The surface interaction probabilities

printed in "Table 2" are calculated as the number of interactions per unit area of the element surface per particle studied. The volume interaction probability calculated is the average path length per particle per unit volume within the volume bounded by the surface of a transparent inner element ( $MREF > 0$ ) and its input and output apertures. Correlation between surface or volume interaction probabilities and "pressure"<sup>(1)</sup> should be applied with caution because of the dependence of "pressure" upon the energy distribution and species of the particles involved.

7.7 The accuracy of the calculated values of surface or volume interaction probability is determined by the number of relevant interactions with the surface in question. The error values quoted with the results are calculated on the basis that the number of events of interest at any particular surface is subject to statistical errors arising from the finite number of particles studied  $N_1$  and the finite number of events at the surface of interest  $N_2$ . If  $N_1$  and  $N_2$  are not too small, the error in  $N_2$  will be<sup>(2,7)</sup>:

$$\pm(1/N_1 + 1/N_2)^{\frac{1}{2}}$$

7.8 Section six of the printout gives the distribution of impact density around the inside surface of each outer element, for primary and sputtered particles, so that the degree of symmetry of particle flow in the structure may be assessed. This is calculated from the division of each outer element into twenty equal segments around the surface and comparing the impact density in each of these with the average impact density for the whole surface given in "Table 2." Since the number of interactions for each of those calculations has been reduced by a factor of 20, in comparison to the number of interactions for the whole surface, the statistical errors of these calculations will be correspondingly large.

7.9 The seventh section gives the distribution of interactions around the inside surface of each outer element for primary and sputtered particles. As in

section six, the elements are divided into 20 equal segments. The table gives the numbers of interactions which have occurred within each segment.

7.10 The eighth and last section of printout gives tables of incidence energies of particles on each surface of each element. The incidence energy is given as a percentage of the energy of primary particles on introduction to the structure. The values relate to the actual number of particles interacting with the surface. By extracting data from these tables, it is possible to determine the energy distribution of primary particles backscattered from any part of the structure. This method was used to determine energy distributions of backscattered particles in the JET "pocket" calculations<sup>(3)</sup>.

## 8. VALIDITY OF THE MODELLING USED IN THE PROGRAM

8.1 Correct operation of the computer program has been checked during development to ensure that modelling of backscattering and sputtering processes gives results which compare favourably with experimental results. Test examples have also been used to check the operation of the various input law distributions.

8.2 The angular distribution of back-scattered primary particles was tested using a copper target structure bombarded with 40keV protons incident at  $45^{\circ}$  with respect to the normal. This incidence angle was obtained by supplying the direction cosines, TAL, TAM and TAN (see section 5.2), such that the trajectory of the primary particles would interact with a small target which was placed at the centre of a large fully adsorbing sphere. The Monte Carlo and experimental angular distributions are shown in Figure 2. The form of the angular distribution obtained seems to be in reasonable agreement with the experimental distribution of 40keV protons backscattered from single crystal copper given by Behrisch<sup>(4,5)</sup>.

8.3 The energy distribution of back-scattered particles was tested using a nickel target bombarded with normally

incident protons at 2.5keV and 7.5keV incidence energies. Normal incidence was achieved in this study by using the isotropic input distribution law with IREF=1. The experimental and Monte Carlo energy distributions for protons incident at 2.5keV and 7.5keV are given in Figures 3 and 4 respectively. The energy distributions obtained from the Monte Carlo calculations are reasonably similar to the experimental distributions given by Eckstein et al<sup>(6)</sup>. The backscattering coefficients obtained from the calculations were also similar to the experimental results<sup>(6)</sup>.

## 9. SOME USEFUL HINTS

9.1 By setting the adsorption threshold energy {THR1} of a surface to a value not less than the primary particle input energy {ENERGY}, a surface can be made fully or partially adsorbing, depending upon the corresponding value of adsorption coefficient {ADS1} (see section 5.7). This technique can be used to override the "multiple scattering model" (Appendix II) when surfaces are to act as "collectors." This method proved extremely useful in the JET "pocket" calculation given in Appendix III where a fully adsorbing hemisphere structure was used to collect particles backscattered from the "pocket" so that angular distribution information could be obtained.

9.2 Sputtering from a surface can be avoided by setting the sputtering threshold energy {STH} of the surface to a value not less than the primary particle input energy {ENERGY} (section 5.8).

9.3 When using open-ended structures, it is sometimes desirable to obtain the energy distributions of particles transmitted or reflected from the structure. This can be achieved by including a transparent diaphragm inner element to cover the open end of the structure. Transparency is obtained by setting MREF > 0 for the element (section 5.6). The energy distribution of particles passing through this diaphragm can be extracted from the tables given in section eight of the printout.

9.4 Structures can be defined to simulate spheres and hemispheres by joining together conical elements of various dimensions. These structures are useful for observing the angular distributions of particles backscattered or sputtered from target structures. Example data for a hemisphere structure is shown in the JET "pocket" test given in Appendix III. The fully adsorbing hemisphere is attached by a diaphragm to the entrance aperture of the cylindrical "pocket" and acts as a collecting plate for particles reflected from the "pocket." The radius of the hemisphere structure is sufficiently greater than that of the cylinder, so that reflected particles appear to originate from the point of origin of the hemisphere. The hemisphere structure is made fully adsorbing and non-sputtering, using the techniques described above. The interaction probabilities for each element of the hemisphere can be plotted against the angle of the surface of the element, measured from the point of origin of the hemisphere, to determine the angular distribution of the particles.

## 10. FUTURE PROGRAM DEVELOPMENT

10.1 In each of the three sections of input data (see section 5), fixed format has been used to aid the user in checking the data. In sections one and three the field lengths of parameters involve more variety than might be desirable. However, in future developments of the program, some thought may be given to standardising the format of the input data to relieve this problem.

10.2 The generation and backscattering of sputtered particles has been restricted in the present version of the program, due to insufficient information being available for accurate simulation of these processes. In the present version, the program has been restricted to dealing with sputtering coefficients no greater than unity and therefore only one sputtered particle may be generated for any one primary particle interaction. Facilities have however been included in the program to handle more than one sputtered particle from any one primary particle interaction, and when techniques

have been developed to deal with sputtering coefficients greater than unity, these facilities will be available for use.

10.3 In the present version of the program, sputtered particles are assumed to be adsorbed at their first interaction, and it is also assumed that they cannot themselves cause further sputtering. During development of the program, facilities were included to handle information about sputtered particles backscattered from surfaces which might also cause further sputtering from those surfaces. As information becomes available, these facilities may be activated to allow the generation of sputtered particles to be more extensively modelled.

10.4 The energy distribution of sputtered particles is as yet undefined and the program disregards the energy of these particles at present. Facilities are included in the program to enable information on the energy of sputtered particles to be handled and as information becomes available these facilities can be activated.

10.5 The present version of the graphical output routine has not yet been modified to include output for sputtered material. The scaling factor given in the graphical output (Appendix IV), is for output on the Benson-Lehrner Model J graph plotter, and has not yet been adjusted for the Calcomp plotter. In future modifications to the program, the graphical output routine could be extended to give interaction probabilities for sputtered material and the scaling factor adjusted to suit the Calcomp plotter.

10.6 Future development of the Monte Carlo computer program will depend largely upon user requirements and comments and suggestions from users will be appreciated.

#### 11. ACKNOWLEDGEMENT

The writer wishes to express his gratitude to J N Chubb who supervised the development of the Monte Carlo program, and to G M McCracken, S K Erents and E S Hotston for encouragement and helpful discussions during the course of this work.

#### REFERENCES

1. Chubb J N. A Monte Carlo computer program for analysis of molecular gas flow. Culham report CLM-R54, 1966.
2. Chubb J N. Monte Carlo studies of free molecular gas flow through various vacuum structures. Proc. 4th Int. Vac. Congress, Manchester, April 1968. Inst. Phys. Conf. Series No 6, p.433.
3. Brown K P. Results of Monte Carlo studies on backscattering and sputtering from "pocket" and "finned" structures. Culham report CLM-R182, January 1978.
4. Behrisch R. Can. J. Phys. 46, p.527-535, 1968.
5. Behrisch R. Rep. Inst. Plasma Phys., 2/68 (Munich Inst. of Plasma Physics, 1968).
6. Eckstein R, Matschke P, Verbeek H. Reflection of hydrogen from stainless steel and Nb. Max-Planck Institute fur Plasmaphysik, Euratom Association, D-8046 Garching bei Munchen, Germany. Paper presented at Int. Conf. Surface Effects in Controlled Fusion Devices, San Francisco, USA, 16-20 February 1976.
7. Chubb J N. Monte Carlo analysis of pumping speed test dome performance for several vapour diffusion pump geometries. Vacuum 16, p.591, 1966.
8. Everhart E, Stone G, Carbone R J. Classical calculation of differential cross section for scattering from a coulomb potential with exponential screening. Phys. Rev. 99, p.1287-90, 1955.
9. Ishitani T and Shimizu R. A simple calculation on backscattering of light ions of KeV energies. Jap.J. Appl. Phys. 10, p.821-826, 1971.
10. Hotston E. Private communication.
11. Behrisch R. First wall erosion in fusion reactors. Nuclear Fusion 12, p.695-713, 1972.
12. McCracken G M. The behaviour of surfaces under ion bombardment. Rep. Prog. Phys. 38, p.241-327, 1975.
13. Bay H L, Roth J. and Bohdansky J. Light ion sputtering yields for molybdenum and gold at low energies. J. Appl. Phys. 48, p.4722-4728, November 1977.

Table 1: Definition of parameters for data card described in section 5.1

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION								
ICASE	1 to 7	Mandatory	<p>This is the number of the case being studied. Since this value also defines the starting point for the random number sequence in the program it is necessary to change ICASE for a second run on a particular structure if any improvement in accuracy is hoped for by the mixing of the two sets of results.</p> <p>ICASE &gt; 999 will cause the necessary instructions to be performed to produce graphical output.</p> <p>ICASE &lt; 0 stops the program.</p>								
IREF	8 to 14	0	<p>This value determines the angular distribution of primary particles entering the structure from the surface defined by INCONE, RINNR, ROUTR, and RCENTR.</p> <p>IREF = 0 gives a cosine input distribution.</p> <p>0 &lt; IREF &lt; 180,000 gives an isotropic distribution into a cone of half angle IREF/1000.</p> <p>IREF &gt; 0 gives input along the positive axis direction and</p> <p>IREF &lt; 0 in the reverse direction.</p> <p>IREF &gt; 180,000 gives a <math>\text{Cos}^2</math> distribution.</p>								
INCONE	15 to 21	1	Number of the length element at whose entrance plane the primary particles are to be introduced.								
RINNR and ROUTR	22 to 35 36 to 49	RI(INCONE) RO(INCONE)	The inner and outer radii of the annular surface from which the primary particle histories start, with random choice of position over the annulus.								
RCENTR	50 to 63	0.0	The displacement of the centre of the annular surface, defined by RINNR and ROUTR, from the system (z) axis along the x direction.								
INAXIS	71 to 72	0	<p>Chooses the direction of the axis along which the primary particles are introduced within IREF choice of distribution.</p> <table> <tr> <td>INAXIS = 0</td> <td>along z axis</td> </tr> <tr> <td>INAXIS = 1</td> <td>along x axis</td> </tr> <tr> <td>INAXIS = 2</td> <td>along y axis</td> </tr> <tr> <td>INAXIS &lt; 0</td> <td>along-z axis</td> </tr> </table> <p>INAXIS = 3 causes the input distribution defined by IREF, RINNR, ROUTR, and RCENTR to be ignored and an extra data card to be read specifying the direction cosines to be used for input to the structure.</p>	INAXIS = 0	along z axis	INAXIS = 1	along x axis	INAXIS = 2	along y axis	INAXIS < 0	along-z axis
INAXIS = 0	along z axis										
INAXIS = 1	along x axis										
INAXIS = 2	along y axis										
INAXIS < 0	along-z axis										

Table 2: Definition of parameters for data card described in section 5.2

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
TAL	1 to 12	Mandatory	These parameters give the direction cosines from the x, y and z axes respectively which are to be assigned to all primary particles on input to the structure. The primary particle histories are started from the (INCON)th element and centred RCENTR from the system axis along the direction of the x axis.
TAM	13 to 24	Mandatory	
TAN	25 to 36	Mandatory	

Table 3: Definition of parameters for data card described in section 5.3

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
NP	1 to 7	Mandatory	The number of primary particle histories to be studied.
IPRINT	8 to 14	Mandatory	The number of primary particle histories to be studied per interval between printing out results.
ENERGY	15 to 26	Mandatory	The energy (eV) of the primary particles on entry to the structure.
IZI	27 to 30	Mandatory	The atomic number of the primary particle species
AM1	31 to 42	Mandatory	The atomic mass of the primary particle species.

Table 4: Definition of parameters for data card described in section 5.4

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
NCS	1 to 7	Mandatory	The number of length elements in the structure.
NADS	8 to 14	Mandatory	The number of sets of adsorption coefficient details used in the structure.
NSUB	15 to 21	Mandatory (maximum 3)	The number of sets of substrate material details used in the structure.

Table 5: Definition of parameters for data card described in section 5.6

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
RI	1 to 4	Mandatory	The radius of the inner surface at the input-end of the element.
RO	15 to 28	Mandatory	The radius of the outer surface at the input-end of the element.
A	29 to 42	Mandatory	The axial length of the element.
MREF	43 to 45	0	MREF = 0 allows scattering and sputtering from the inside and outside of the inner surface. MREF > 0 makes the inner surface transparent so that particle trajectories pass through undeflected. The number of interactions on transparent surfaces are recorded and used to calculate the volume interaction probability for the inner elements as described in section 7.6
IADSI	46 to 48	Mandatory	Index number of adsorption details for inside of inner element.
IADSOI	49 to 51	Mandatory	Index number of adsorption details for outside of inner element.
IADSAO	52 to 54	Mandatory	Index number of adsorption details for inside of outer element.
I SUBII	55 to 57	Mandatory	Index number of substrate details for inside of inner element.
I SUBOI	58 to 60	Mandatory	Index number of substrate details for outside of inner element.
I SUBAO	61 to 63	Mandatory	Index number of substrate details for inside of outer element.

At the end of the sequence describing the above parameters for all NCS elements of the structure, there must be a further data card giving the output-side radii of the last element, RI (NCS+1) and RO (NCS+1) in (2 F14.7) format.

Table 6: Definition of parameters for data card described in section 5.7

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
IADS	1 to 3	Mandatory	The index number of this set of adsorption details. This number corresponds to one of the index numbers defined by IADSI, IADSOI and IADSAO.
ADS1	4 toll	Mandatory	The adsorption coefficient for all surfaces with index number IADS.
THRL	12to23	Mandatory	The threshold energy (eV) below which the adsorption coefficient becomes effective. Primary particles with energy greater than THRL will penetrate into the solid and be followed using the "multiple scattering model." (See Appendix II).

Table 7: Definition of parameters for data card described in section 5.8

PARAMETER	CARD COLUMNS	DEFAULT VALUE	DESCRIPTION
ISUB	1 to 4	Mandatory	The index number for this set of substrate details. This number corresponds to one of the index numbers defined by ISUBII, ISUBOI and ISUBAO.
IZA1	5 to 8	Mandatory	The atomic number of the incident primary particle species. This number should correspond with the value IZ1 (see section 5.3).
IZA2	9 tol2	Mandatory	The atomic number of the substrate material for all surfaces with substrate index number ISUB.
AMASS	13to20	Mandatory	The atomic mass of the substrate material.
ADEN	21to28	Mandatory	The density ( $\text{GM.cm}^{-3}$ ) of the substrate material.
RNGE and RNEN	29to34 35to46	Mandatory Mandatory	RNGE is the range (microns) of the primary particle species incident on the substrate with energy RNEN (eV). From these values the program calculates the range for any given incidence energy.
STH	47to58	Mandatory	The sputtering threshold energy (eV). Sputtering of the substrate material can only occur when the energy of the incident primary particle is greater than STH.
EMP1 and EMP2	59to70 71to77	Mandatory Mandatory	Empirical values A and B respectively used in the sputtering equation (see Appendix II). Typical values (for $\text{H}^+$ on Mo) are $8.99 \times 10^{-3}$ and 0.017 respectively.

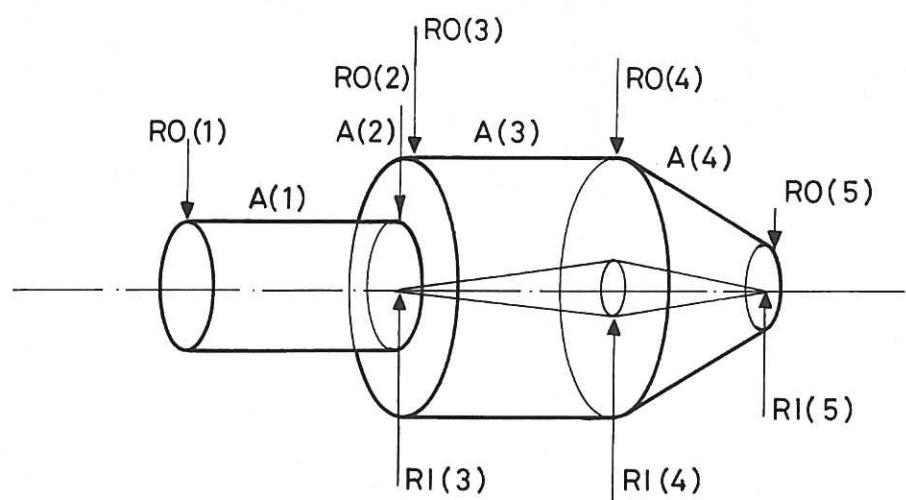


Fig.1 The general form of the structure handled by the program.

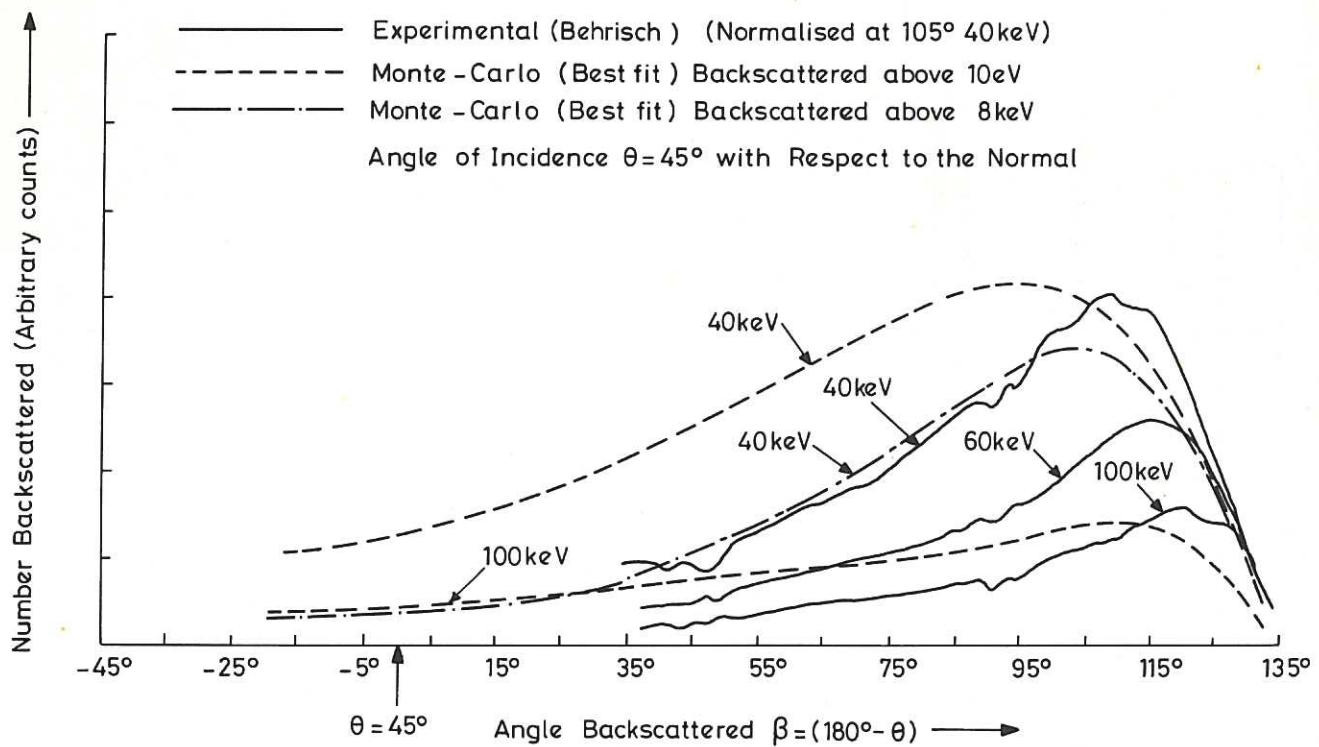


Fig.2 Angular distribution of backscattered particles for  $H^+$  incident on copper at  $45^\circ$  with respect to the normal.

CLM-R181

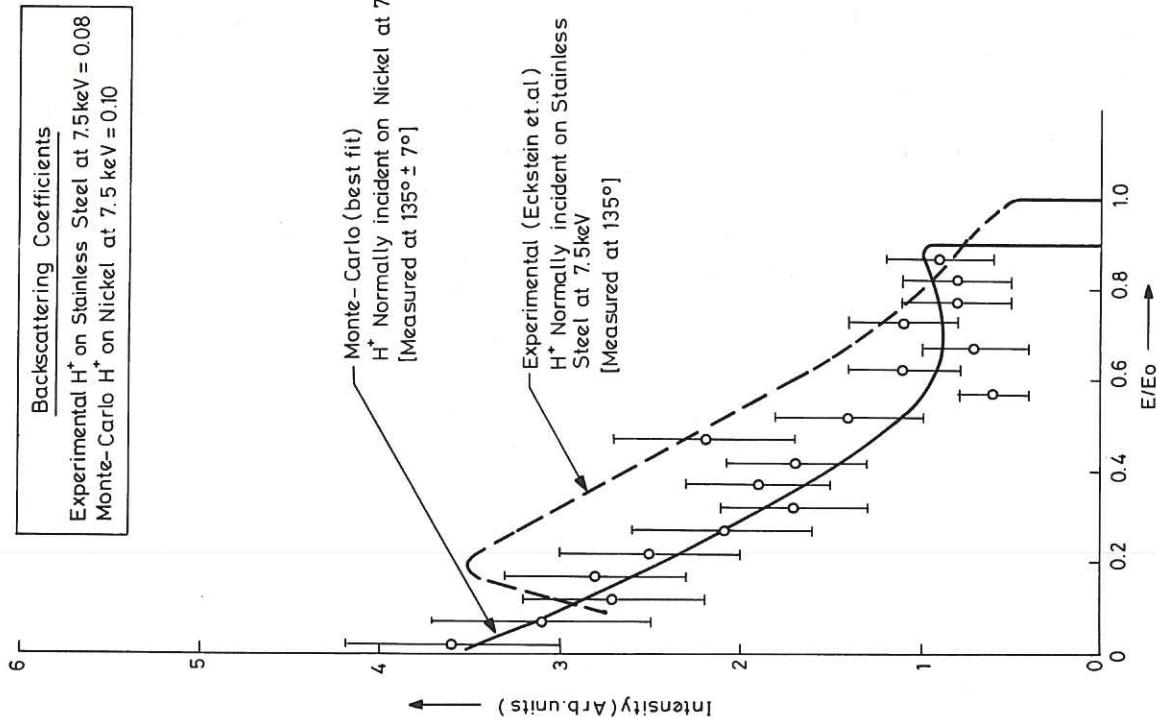
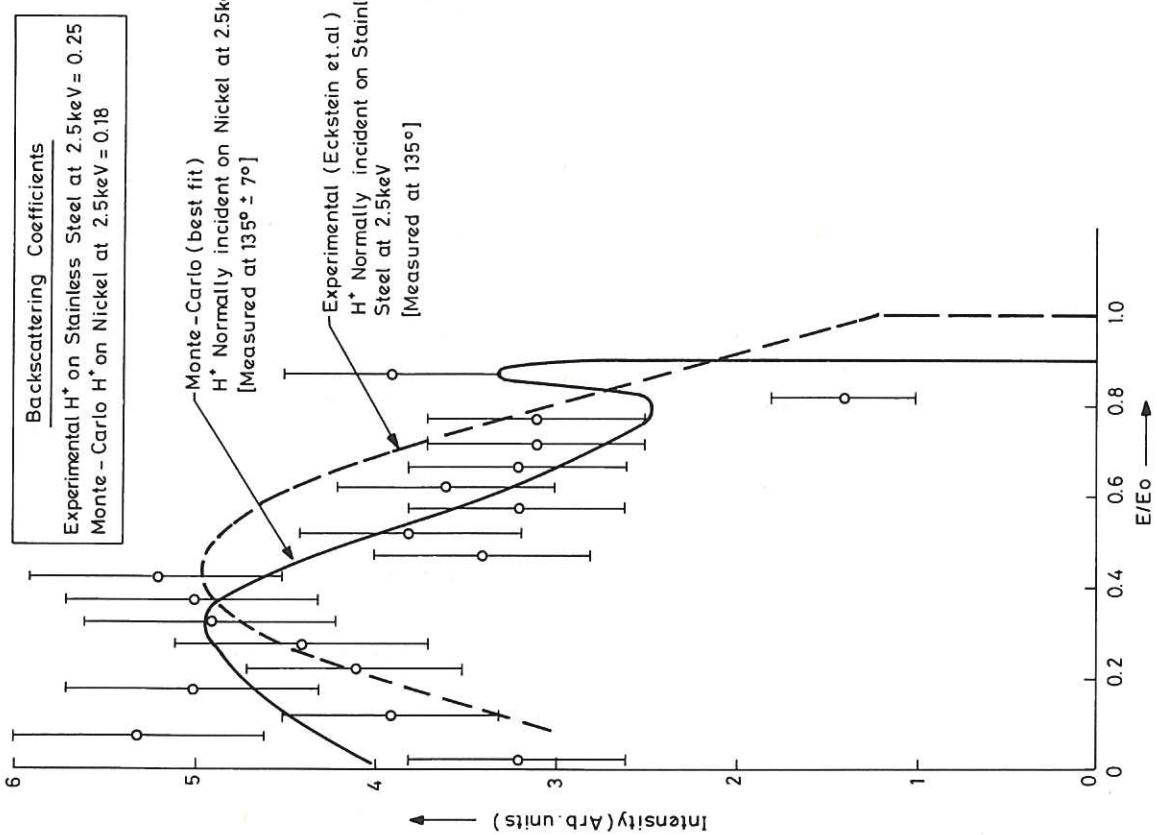


Fig.3 Energy spectra of backscattered particles for  $H^+$  incident normally on stainless steel and nickel at 2.5 keV.

Fig.4 Energy spectra of backscattered particles for  $H^+$  incident normally on stainless steel and nickel at 7.5 keV.

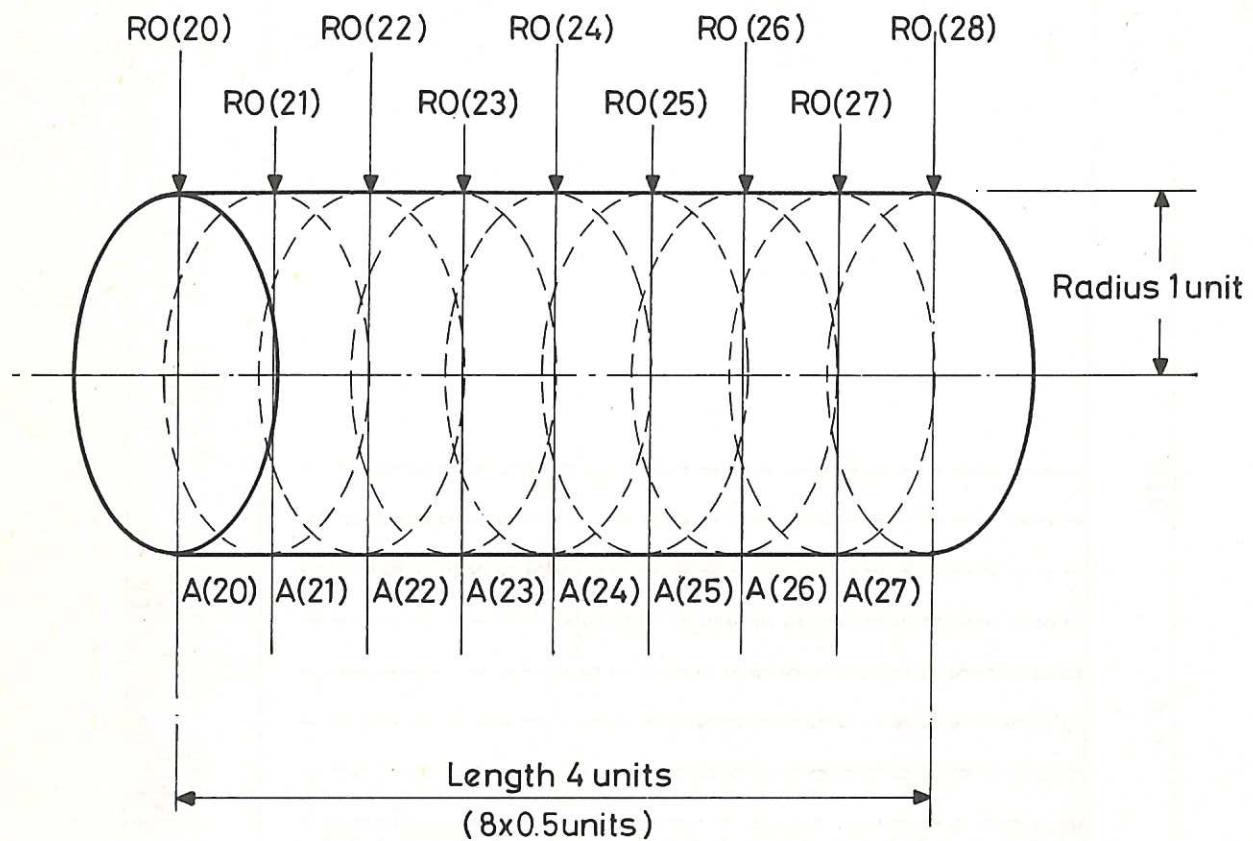


Fig.5 The cylindrical "pocket" structure used in the JET calculations.

CLM-R 181

```
// LOGIN ABCDEF,123456  
// REPLACE ABCDEF:FRED.DATA(50010)
```

COMMENTS

		19	0	1	0.0	1.0	1.0	0.0	0	0	Data section 1
1011	0	0.0	0.0	0.0	0.5	0	2	2	2	2	Data section 2
2000	2000	1000.0	1	0.0	0.5	0	2	2	2	2	
28	2	2	0.0	0.0	0.0	0.5	0	2	2	2	
			0.0	0.0	0.0	0.0	0	2	2	2	
			10.0	0	0.5	0	2	2	2	2	
			14.107	1.0	0	0	2	2	2	2	
			19.647	2.0	0	0	2	2	2	2	
			28.0	2.0	0	0	2	2	2	2	
			34.118	2.0	0	0	2	2	2	2	
			39.191	2.0	0	0	2	2	2	2	
			43.589	2.0	0	0	2	2	2	2	
			52.689	2.0	0	0	2	2	2	2	
			64.0	10.0	0	0	2	2	2	2	
			71.414	10.0	0	0	2	2	2	2	
			80.0	10.0	0	0	2	2	2	2	
			86.6	10.0	0	0	2	2	2	2	
			91.652	10.0	0	0	2	2	2	2	
			95.39	10.0	0	0	2	2	2	2	
			97.98	10.0	0	0	2	2	2	2	
			99.499	10.0	0	0	2	2	2	2	
			100.0	0.0	0.0	0.0	0	2	2	2	
			100.0	1.0	0	0.0	0	1	1	1	
			0.0	0.0	0.0	0.0	0	2	2	2	
			0.0	1.0	0	0.0	0	1	1	1	
			0.0	0.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
			0.0	1.0	0.5	0	1	1	1	1	
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2	1.0	1000.0	0	0	0.30	10000.000	100000.000	8.99D+3	0.017	0.017	Data section 3
1	1.42	96.00	10.2	0.30	10000.000	10000.000	170.000	8.99D+3	0.017	0.017	
2	1.42	96.00	10.2	0.30	10000.000	10000.000	170.000	8.99D+3	0.017	0.017	
** CYLINDRICAL POCKET = RATIO L/D=2/1 = H ON NO AT 1KEV *											
											Terminator

```
/*  
// LOGOUT  
// ENDIPT
```

Fig.6 The data file for the cylindrical "pocket" calculations.

```

// LOGIN ABCDEF,123456
// REPLACE ABCDEF:FRED.RUNJET(S)-
// SCHEDULE JNCMCO:KEITH.MC08,250,101
// CONFG RSP=2G09,STORE=470
// FILE DSET97,RA,ABCDEF:FRED.DATA(S0010)
// FILE GRIDFL,RA,ABCDEF:FRED.GRAPHS(N0010)
// EXEC ABCDEF:FRED.DSET99(S)
/*
// LOGOUT
// ENDIPT

```

Fig.7 The procedure file for running the Monte Carlo program.

Notes:

1. The user's own username and password must be supplied for LOGIN.
2. File-identifiers, except for the program-name JNCMCO:KEITH, MC08 should be replaced by the user's own specifications.

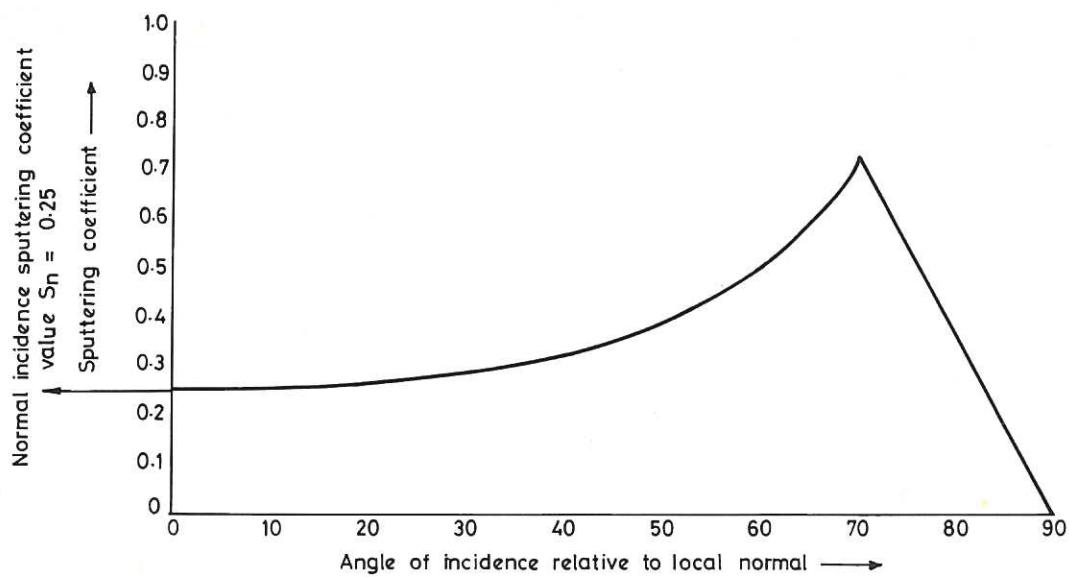
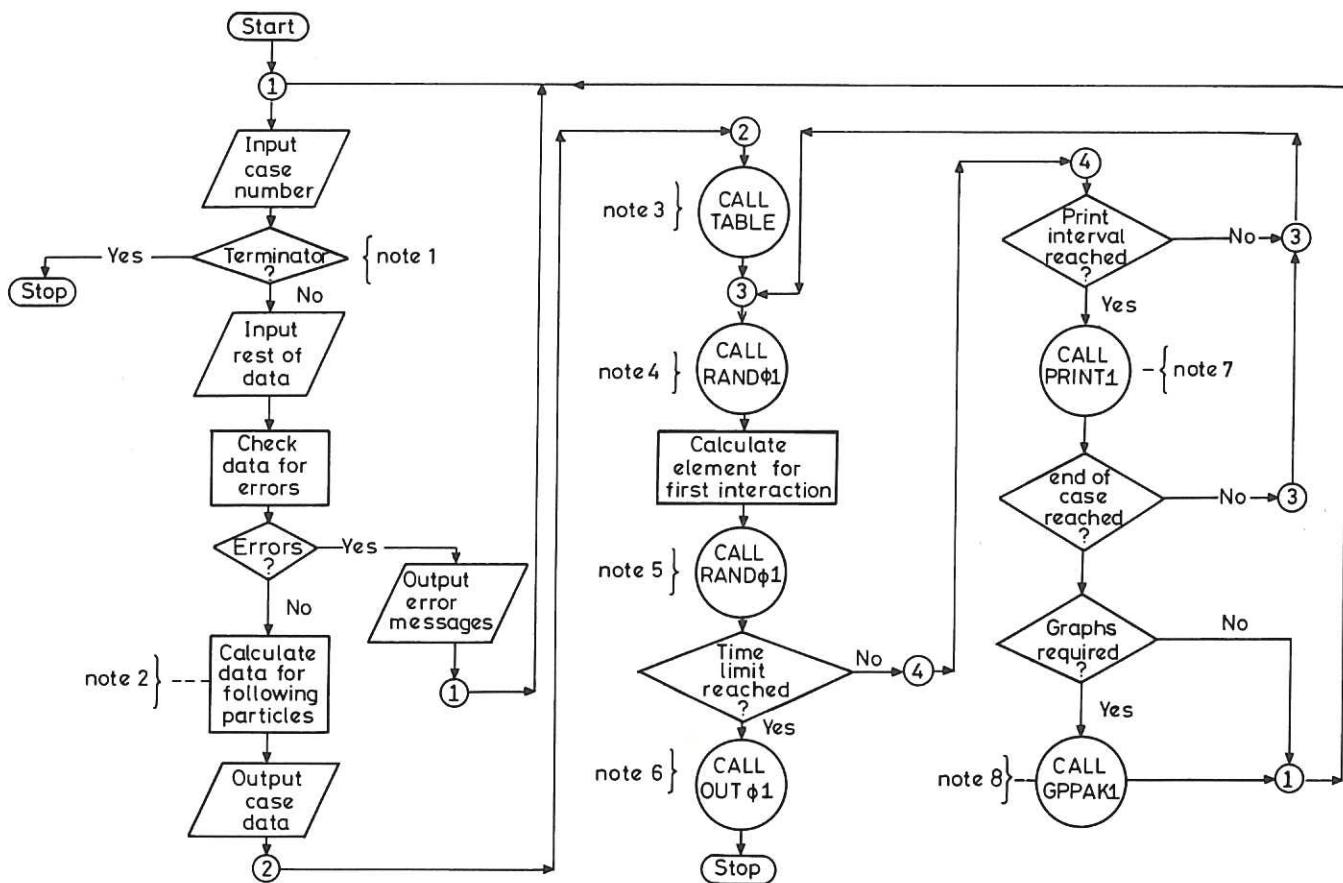


Fig.8 Variation of sputtering coefficient with angle of incidence.





Outline Flowchart of Monte-Carlo Program — Main Segment. Routine MAINØ8(F).

1. A negative case number indicates the end of input data.
2. Data required for following particle trajectories includes the distance to the cone apex and the sine and cosine of the cone half angle for each length element of the structure.
3. Segment TABLE - routine TABLE8(F) - is used to set up tables of direction cosines of angles of deflection for use in the "multiple scattering model" for following primary particles through the substrate.
4. Segment RANDØ1 - routine RANDØ8(F) - is used to generate direction cosines within a given distribution for primary particles entering the structure at a given entrance plane.
5. Segment RINGØ1 - routine RINGØ8(F) - is used to follow each primary particle history through the structure. RINGØ1

calls other routines to determine sputtering, backscattering and adsorption on interaction with any element of the structure. When sputtered particles are generated, RINGØ1 follows their histories through the structure before returning to follow the primary particles.

6. Segment OUTØ1 - routine OUTØ8(F) - is used when insufficient time is left to follow another primary particle history. This routine calls segments PRINT1 and GPPAK1 to output results before terminating the program.

7. Segment PRINT1 - routine PRINT8(F) - is used to evaluate and output statistical results after each print interval and when "timeout" occurs.

8. Segment GPPAK1 - routine GRAFØ8(F) - is used to plot the structure and interaction probabilities for each case studied. This routine is only called when case number > 999.



## Appendix II Outline description of program operation

### 1. Introduction

1.1 Primary particles are input to the structure within a chosen input area, with a chosen input angular distribution and with a chosen energy and atomic mass and number. On interaction with a surface in the structure, the program uses Monte Carlo techniques to determine whether or not a sputtered particle is generated from that surface. If a sputtered particle is generated, it is assigned an energy and direction cosines using Monte Carlo techniques. This sputtered particle is identified by the atomic mass and number of the surface from which it is generated. The direction cosines and co-ordinates of the incident particles are temporarily saved in a table, and the path of the sputtered particle is followed until the particle is adsorbed on a surface or exits from the structure. When the history of the sputtered particle is terminated, the program returns to study the incident species particle. The incident particle is followed through a series of nuclear collisions within the substrate material until it is either adsorbed or is backscattered from the surface with a reduced energy and new direction cosines. If backscattering occurs, the incident particle is followed until its next interaction with a surface, and again sputtering is examined. The incident particle history is terminated when the particle is adsorbed on a surface or exits from the structure. When the primary particle history is terminated, another primary particle is input to the structure and studied. When a suitable number of primary particles have been studied, the program terminates the study of the structure.

### 2. Backscattering

2.1 The backscattering of primary particles is determined by a "multiple scattering model." The particle is followed through a series of nuclear collisions in the solid until it is adsorbed or is backscattered to the surface with a reduced energy and new direction cosines. Adsorption occurs when the primary particle energy has reduced to such a value that it cannot escape back to the surface.

2.2 The particle trajectory in the substrate is considered in terms of a series of steps with the length of each step adjusted so that the maximum value of the scattering impact parameter does not cause an angular deflection greater than  $20^{\circ}$ . The actual value of the impact parameter for interaction in a step length is determined by random number choice. The angle of deflection at scattering events is calculated using an exponentially screened Coulomb field model<sup>(8)</sup>.

#### Screening length

$$a = a_0 / \{Z_1^{2/3} + Z_2^{2/3}\}^{1/2} \quad (1)$$

where  $a_0$  is the Bohr radius and  $Z_1$  and  $Z_2$  are the atomic numbers of the incident and target atoms respectively.

#### Collision diameter

$$b = Z_1 Z_2 e^2 / (\frac{1}{2} m v^2) \quad (2)$$

where  $e$  is the electron charge (e.s.u.).

### Angle of deflection

$$\theta = 2 \cot^{-1} \left\{ \frac{2p/b}{\exp(-1/Z_0)} \right\} + \frac{2p}{a} Z_0 \int_0^{\infty} (y_0^{-\frac{1}{2}} - y^{-\frac{1}{2}}) dz \quad (3)$$

$$y = 1 - (p/a)^2 z^2 - (b/a)z \exp(-1/z) \quad (4)$$

$$y_0 = 1 - (p/a)^2 z^2 - (b/a)z \exp(-1/Z_0) \quad (5)$$

where  $p$  is the impact parameter and  $Z_0$  is the root of equation (4).

The angle of deflection  $\theta$  is in "centre of mass system" and is converted back into "Laboratory system" by the program.

2.3 The calculation of the angle of deflection using equation (3) proved to be extremely time consuming. To reduce the calculation time a look-up table approach has been adopted with linear interpolation between the nearest neighbour values in the table. An example look-up table of direction cosines of angular deflections for a range of impact parameters and incidence energies is shown in section two of the printout given in Appendix IV. At each nuclear collision the program enters the table for the substrate material involved with the energy and impact parameter of the incident particle and returns with the angle of deflection. The impact parameter is chosen using Monte Carlo techniques. The new direction cosines and the depth of the particle in the solid are calculated and the trajectory followed until the particle is either backscattered or adsorbed.

2.4 As the primary particle is followed in the solid, its energy is reduced due to the effect of "electronic stopping." The energy of the particle after moving through a given distance is given by Ishitani and Shimizu<sup>(9)</sup> as:

$$E(y) = E_0 (1-y)^2 \quad (6)$$

$E_0$  is the energy of the primary particle on interaction, and  $y$  is obtained from:

$$y = x/R \quad (7)$$

where  $x$  is the distance travelled in the solid and  $R$  is the range of the particle at interaction with the surface.

The range  $R$  is input as a parameter with the structure data for the program.

2.5 The energy of the primary particle is also reduced by "nuclear stopping" where particles undergo a significant deflection - which in our model is above 20°.

The equation used by Ishitani and Shimizu<sup>(9)</sup> for the energy of the primary particle after a nuclear collision is given as:

$$E = C^2 E_0 \quad (8)$$

where  $C = \frac{-A \cos \theta + (1 - A^2 \sin^2 \theta)^{\frac{1}{2}}}{1 + A}$  (9)

and  $A = \frac{M_1}{M_2}$  (10)

Here  $\theta$  is the angle of deflection in the Laboratory system and  $M_1$  and  $M_2$  are the atomic masses of the incident and target atoms respectively.

2.6 The interpolation on the tables of angles of incidence, and the generation of the tables themselves (2.2), has so far been based on only one incident and one substrate

material ( $H^+$  on Mo). Further investigation of the interpolation method and the mesh structure of the tables may be needed to cater for other materials as well as to improve accuracy in certain regions of the tables.

### 3. Sputtering

3.1 When a primary particle interacts with a surface, the program checks if sputtering of the substrate material has occurred. The equation used for calculating the sputtering coefficient for normal incidence angles as a function of incident energy and substrate material is given by Hotston<sup>(10)</sup> as:

$$s = \frac{A}{\left\{ \frac{E}{2} + \left\{ \frac{2}{E - E_c} \right\}^2 \right\}^{1/2}} \exp(-0.017 E) \quad (11)$$

where  $E$  is the incident energy (keV)

$E_c$  is the threshold energy (0.17 keV for Mo)  
and  $A$  is a variable ( $8.99 \times 10^{-3}$  for Mo)<sup>†</sup>

For primary particles with energy above the threshold energy ( $E_c$ ) the program calculates the normal incidence value of sputtering coefficients from equation (11). Using this sputtering coefficient the program calculates the probability of a sputtered particle being generated as a function of the incidence angle of the primary particle. For incidence angles below  $70^\circ$  with respect to the normal, the probability of sputtering  $p$  is calculated as:

$$p = s/\cos \theta \quad (12)$$

where  $s$  is the sputtering coefficient at normal incidence and  $\theta$  is the angle of incidence.

Equation (11) models the curve given by Behrisch<sup>(11)</sup> for sputtering of polycrystalline Nb by light ions. It is assumed that this equation also models sputtering yields for Mo.<sup>†</sup>

For angles ( $\theta$ ) up to  $70^\circ$  with respect to the normal, McCracken<sup>(12)</sup> suggests a  $(\cos \theta)^{-1}$  relationship. The variation for angles above  $70^\circ$  is still uncertain and for our model we have chosen an arbitrary linear relationship reducing from a peak at  $70^\circ$  to zero at grazing incidence. The overall form of variation of sputtering coefficients with incidence angle, as used in the present program, is shown in Figure 8.

For angles above  $70^\circ$  a linear relationship is used, as:

$$p = \cos \theta \cdot s/\cos^2 \beta \quad (13)$$

where  $\beta$  is  $70^\circ$ .

The decision on whether a sputtered particle is generated or not at any particular interaction of a primary particle with a surface is based on the choice of a random number and comparison of the number obtained to the value of  $p$  derived as above.

3.2 Although the program at present only allows one sputtered particle to be generated at any one interaction of the primary particle, facilities are included to follow more

---

<sup>†</sup>Recent studies by Bay et al<sup>(13)</sup> for  $H^+$  incident normally on Mo indicate that sputtering coefficients may be around a factor of 3 lower than obtained from equation (11) with the parameter values quoted. More accurate modelling of  $H^+$  on Mo should be achieved by reducing the empirical value  $A$  to around  $3.0 \times 10^{-3}$ . This parameter is read into the program as EMPL (see Table 7, and section 5.8).

than one sputtered particle generated from any interaction. The program also assumes at the moment that all sputtered particles will be adsorbed at their first interaction with a surface, and the sputtered particles cannot themselves cause sputtering. The program has facilities to allow sputtered particles to be backscattered on interactions with surfaces and to cause further sputtering from those surfaces. As information becomes available these facilities can be activated to allow the generation of sputtered particles to be more accurately modelled.

3.3 The energy distribution of sputtered particles is as yet undefined, and the program disregards the energy of these particles at present. In further development of the program, it may be desirable to give the energy distribution of sputtered particles. The angular distribution of sputtered particles is at present assumed to be cosine but alternative distributions could be implemented if information is available.

Appendix III. Example run of Monte Carlo program

The example given here was used in the "pocket" calculations performed for JET<sup>(3)</sup>. The aim of this particular calculation was to determine the amount of backscattered and sputtered material reflected from a cylindrical "pocket" structure of length to diameter ratio 2:1 when bombarded with protons with energy of 1keV. The backscattering and sputtering coefficients obtained for this structure could then be compared with results for a "plane surface" structure to determine the reduction in flux of backscattered particles and sputtered material achieved by the "pocket" structure.

The "pocket" structure used in this calculation is illustrated in Figure 5. The "pocket" is made up of several equal length elements so that the printed results will give some idea of the distribution of interactions and adsorptions within the "pocket". A fully adsorbing hemisphere structure was attached to the input-end orifice of the "pocket" by a diaphragm and another diaphragm was used to close the output-end orifice of the structure. This resulted in a fully closed structure with the hemisphere acting as a collector for particles reflected from the "pocket," enabling angular and energy distribution to be extracted from the printed results.

The primary particles (protons) were introduced uniformly over the entrance aperture of the "pocket" INCONE = 19 - within a cosine distribution of incidence angles - IREF = 0 - and with energy of 1keV - ENERGY = 1000.0.

The card deck for setting up the data file for this calculation is given in Figure 6. The procedure file containing the necessary job control statements for running the program is given in Figure 7.

The job is submitted to the job queue by issuing the following commands:

```
//LOGIN ABCDEF,123456
//REMJOB ABCDEF:FRED.RUNJET(S)
//LOGOUT
//ENDIPT
```

When the job has been run, the graphical output file - ABCDEF:FRED.GRAPHS(NØØ1Ø) - is submitted for processing by issuing the following commands:

```
//LOGIN ABCDEF,123456
//GRAPHS NARROW,ABCDEF:FRED.GRAPHS(NØØ1Ø)
//LOGOUT
//ENDIPT
```

The results obtained from this calculation are given in Appendix IV.

Notes

1. The username and password together with file-identifiers used throughout this example should be replaced by the user's own specifications.
2. New users of Multijob should refer to the "Multijob Using Remote Terminals" manual for further information on running jobs and setting up files.



## Appendix IV

IN THE TABLE LISTING THE DISTRIBUTION OF ADSORPTIONS AND INTERACTIONS THE SURFACE INTERACTION PROBABILITIES ( $DMNAI(i)$ ) AND ( $DMNAO(i)$ ) ARE CALCULATED AS THE NUMBER OF INTERACTIONS OCCURRING IN THE ( $i$ )TH ELEMENT PER UNIT SURFACE AREA OF THE ELEMENT PER PARTICLE INTRODUCED INTO THE SYSTEM.

IF THE STRUCTURAL DIMENSIONS ARE IN INCHES THEN ( $DMNAI(i)$ ) OR ( $DMNAO(i)$ ) MULTIPLIED BY THE NETT GAS FLOW INTO THE STRUCTURE IN LITRE.TORR PER SEC. AND DIVIDED BY 264.0 GIVES THE PRESSURE AT THE ( $i$ )TH ELEMENT IN TORR. FOR HYDROGEN

THE VOLUME INTERACTION PROBABILITY IS THE AVERAGE PATH LENGTH PER UNIT VOLUME OF THE INNER ELEMENT PER MOLECULE ENTERING THE SYSTEM. ASSUMING AMBIENT TEMPERATURE MOLECULAR ENERGIES THE EFFECTIVE PRESSURE IN TORR WILL BE  
(VOLUME INTERACTION PROBABILITY)\*(GAS INFLOW(T.L.SEC-1))/G  
WHERE G=1140 FOR HYDROGEN, 304 FOR NITROGEN, AND 250 FOR ARGON.

MONT CARLO PROGRAM 4 ON 4-70 (10.1270 )

CASE NUMBER 1011 20:13:23 31/08/77

MOLECULAR HISTORIES INITIATED AT ENTRANCE PLANE OF NUMBER 19 CONE  
FROM ANNULAR SURFACE BETWEEN RADII 0.0000000 AND

1.0000000 CENTERED 0.0000000 FROM THE SYSTEM AXIS ALONG X AXIS

WITH INPUT ENERGY OF 1000.000 EV

COSINE INPUT LAW

ALONG THE DIRECTION OF THE Z AXIS.

COSINE REFLECTION LAW

ATOMIC NUMBER OF PRIMARY PARTICLES = 1  
ATOMIC MASS OF PRIMARY PARTICLES = 1.000

INPUT TABLE

COMPONENT NO.	INNER RADIUS	OUTER RADIUS	LENGTH	MREF	---ADSORBTION INDEX NO.---			---SUBSTRATE INDEX NO.---		
					(II)	(OI)	(AO)	(II)	(OI)	(AO)
1	0.0000000	0.0000000	0.5000000	0	2	2	2	1	1	1
2	0.0000000	10.0000000	0.5000000	0	2	2	2	1	1	1
3	0.0000000	14.1070000	1.0000000	0	2	2	2	1	1	1
4	0.0000000	19.6470000	2.0000000	0	2	2	2	1	1	1
5	0.0000000	28.0000000	2.0000000	0	2	2	2	1	1	1
6	0.0000000	34.1180000	2.0000000	0	2	2	2	1	1	1
7	0.0000000	39.1910000	2.0000000	0	2	2	2	1	1	1
8	0.0000000	43.5890000	5.0000000	0	2	2	2	1	1	1
9	0.0000000	52.6890000	5.0000000	0	2	2	2	1	1	1
10	0.0000000	60.0000000	10.0000000	0	2	2	2	1	1	1
11	0.0000000	71.4140000	10.0000000	0	2	2	2	1	1	1
12	0.0000000	80.0000000	10.0000000	0	2	2	2	1	1	1
13	0.0000000	86.6600000	10.0000000	0	2	2	2	1	1	1
14	0.0000000	91.6520000	10.0000000	0	2	2	2	1	1	1
15	0.0000000	95.3900000	10.0000000	0	2	2	2	1	1	1
16	0.0000000	97.9800000	10.0000000	0	2	2	2	1	1	1
17	0.0000000	99.4990000	10.0000000	0	2	2	2	1	1	1
18	0.0000000	100.0000000	0.0000000	0	2	2	2	1	1	1
19	0.0000000	1.0000000	0.0000000	0	1	1	1	2	2	2
20	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
21	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
22	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
23	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
24	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
25	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
26	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
27	0.0000000	1.0000000	0.5000000	0	1	1	1	2	2	2
28	0.0000000	1.0000000	0.0000000	0	1	1	1	2	2	2
	0.0000000	0.0000000								

TABLE OF ADSORBTION DETAILS

INDEX NO.	ADSORBTION COEFFICIENT	THRESHOLD ENERGY (EV)
1	0.00000	0.000
2	1.00000	10000.000

TABLE OF SUBSTRATE DETAILS

INDEX NO.	ATOMIC NUMBER	ATOMIC MASS	DENSITY (GM.CM-3)	RANGE (MICRONS)	ENERGY (EV) AT RANGE	SPUTTERING THRESHOLD ENERGY (EV)	EMPIRICAL VALUES FOR SPUTTERING EQUATION (EMPA)	EMPIRICAL VALUES FOR SPUTTERING EQUATION (EMPB)
1	42	96.000	10.200	0.30	10000.000	10000.000	0.8990D-02	0.0170
2	42	96.000	10.200	0.30	10000.000	170.000	0.8990D-02	0.0170

TOTAL LENGTH OF STRUCTURE IS 104.400000 UNITS

WZ1 = 1.0

WM1 = 1.0

WZ2 = 42,0

WM2 = 96.0

WZ1= 1.0 WH1= 1.0 WZ2= 42.0 WM2= 96.0

WZ1 = -1.0

WM1= -1,0

WZ2 = 42.0

W.M.2 = -96.0

WZ1= 1.0 WM1= 1.0 WZ2= 42.0 WM2= 96.0

TOTAL SURFACE AREA OF OUTER ELEMENTS IS 94223.5191793 LENGTH UNITS SQUARED

OUTPUT FROM IC-4 CASE NUMBER 1011 CALCULATION PERFORMED 20:27:34 31/08/77

PRIMARY PARTICLES				SPUTTERED PARTICLES			
PARTICLES	DISPERSION	PROBABILITY	P/C ERROR	PARTICLES	DISPERSION	PROBABILITY	P/C ERROR
ADSORPTIONS 2000	0.0000000	1.0000000	0.0000000	14	0.0000000	1.0000000	0.0000000
TRANSMISSIONS 0	0.0000000	0.0000000	0.0000000	0	0.0000000	0.0000000	0.0000000
REFLECTIONS 0	0.0000000	0.0000000	0.0000000	0	0.0000000	0.0000000	0.0000000
TOTAL NUMBER OF PRIMARY PARTICLES STUDIED 2000							
TOTAL NUMBER OF SPUTTERED PARTICLES STUDIED 14							

TABLE 1 DISTRIBUTION OF ADSORPTIONS AND INTERACTIONS

PRIMARY PARTICLES				SPUTTERED PARTICLES			
ELEMENT NO.	ADSORPTIONS	INTERACTIONS	ADSORPTION INDEX NO.	SUBSTRATE INDEX NO.	GENERATED	ADSORPTIONS	INTERACTIONS
(1)	(LNII(I))	(MNII(I))	(IADSII(I))	(ISUBII(I))	(NSPLII(I))	(LNSII(I))	(MNSII(I))
	(LHOI(I))	(MHOI(I))	(IADSOI(I))	(ISUBOI(I))	(NSPLOI(I))	(LNSOI(I))	(MNSOI(I))
	(LNAO(I))	(MNAO(I))	(IADSAO(I))	(ISUBAO(I))	(NSPLAO(I))	(LNSAO(I))	(MNSAO(I))
1	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
2	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
3	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	5	5	2	1	0	0	0
4	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	10	10	2	1	0	1	1
5	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	13	13	2	1	0	0	0
6	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	7	7	2	1	0	0	0
7	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	13	13	2	1	0	0	0
8	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	30	30	2	1	0	0	0
9	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	26	26	2	1	0	0	0
10	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	53	53	2	1	0	0	0
11	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	54	54	2	1	0	0	0
12	0	0	2	1	0	0	0
	0	0	2	1	0	0	0
	33	33	2	1	0	0	0

13	0 0 40	0 0 40	2 2 2	1 1 1	0 0 0	0 0 0	0 0 0
14	0 0 31	0 0 31	2 2 2	1 1 1	0 0 0	0 0 1	0 0 1
15	0 0 29	0 0 29	2 2 2	1 1 1	0 0 0	0 0 0	0 0 0
16	0 0 15	0 0 15	2 2 2	1 1 1	0 0 0	0 0 0	0 0 0
17	0 0 1	0 0 1	2 2 2	1 1 1	0 0 0	0 0 0	0 0 0
18	0 0 0	0 0 0	2 2 2	1 1 1	0 0 0	0 0 0	0 0 0
19	0 0 0	0 0 0	1 1 1	2 2 2	0 0 0	0 0 0	0 0 0
20	0 0 406	0 0 1025	1 1 1	2 2 2	0 0 6	0 0 2	0 0 2
21	0 0 305	0 0 701	1 1 1	2 2 2	0 0 2	0 0 4	0 0 4
22	0 0 189	0 0 525	1 1 1	2 2 2	0 0 2	0 0 0	0 0 0
23	0 0 169	0 0 416	1 1 1	2 2 2	0 0 2	0 0 3	0 0 3
24	0 0 126	0 0 312	1 1 1	2 2 2	0 0 0	0 0 1	0 0 1
25	0 0 98	0 0 233	1 1 1	2 2 2	0 0 1	0 0 1	0 0 1
26	0 0 80	0 0 226	1 1 1	2 2 2	0 0 0	0 0 1	0 0 1
27	0 0 105	0 0 226	1 1 1	2 2 2	0 0 0	0 0 0	0 0 0
28	0 0 162	0 0 356	1 1 1	2 2 2	0 0 1	0 0 0	0 0 0

TABLE 2 DISTRIBUTION OF INTERACTION PROBABILITIES

PRIMARY PARTICLES				SPUTTERED PARTICLES			
ELEMENT NO.	INTERACTIONS	SURFACE INTERACTION PROB.	VOLUME INTERACTION PROB.	INTERACTIONS	SURFACE INTERACTION PROB.	VOLUME INTERACTION PROB.	
(1)	(MNII(1))	(DMNII(1))	(DNIII(1))	(MNSII(1))	(DMNSII(1))	(DMNSII(1))	
	(MNOI(1))	(DMNOI(1))	(DINOI(1))	(MNSOI(1))	(DMNSOI(1))	(DMNSOI(1))	
	(HNAO(1))	(DMAAO(1))	(DHNAO(1))	(MNSAO(1))	(DMNSAO(1))	(DMNSAO(1))	
1	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	+ -	0.000000000		+ -	0.000000000		
2	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	+ -	0.000000000		+ -	0.000000000		
3	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	5	0.000004186		0	0.000000000		
	+ -	0.000001875		+ -	0.000000000		
4	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	10	0.000003387		1	0.000055532		
	+ -	0.000001232		+ -	0.000057481		
5	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	13	0.000005172		0	0.000000000		
	+ -	0.000001439		+ -	0.000000000		
6	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	7	0.000002785		0	0.000000000		
	+ -	0.000001054		+ -	0.000000000		
7	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	13	0.000005169		0	0.000000000		
	+ -	0.000001438		+ -	0.000000000		
8	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	30	0.000004772		0	0.000000000		
	+ -	0.000000378		+ -	0.000000000		
9	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	26	0.000004142		0	0.000000000		
	+ -	0.000000318		+ -	0.000000000		
10	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	53	0.000004226		0	0.000000000		
	+ -	0.000000588		+ -	0.000000000		
11	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	54	0.000004302		0	0.000000000		
	+ -	0.000000593		+ -	0.000000000		
12	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	33	0.000002621		0	0.000000000		
	+ -	0.000000460		+ -	0.000000000		
13	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	40	0.000003192		0	0.000000000		
	+ -	0.000000510		+ -	0.000000000		
14	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	31	0.000002469		1	0.000011379		
	+ -	0.000000447		+ -	0.000011778		
15	0	0.000000000		0	0.000000000		
	0	0.000000000		0	0.000000000		
	29	0.000002310		0	0.000000000		
	+ -	0.000000432		+ -	0.000000000		

16	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
15	0.000001195	+ - 0.000000310	0	0.000000000
			+	0.000000000
17	0	0.000000000.	0	0.000000000
	0	0.000000000	0	0.000000000
1	0.000000080	+ - 0.000000080	0	0.000000000
			+	0.000000000
18	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
0	0.000000000	+ - 0.000000000	0	0.000000000
			+	0.000000000
19	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
0	0.000000000	+ - 0.000000000	0	0.000000000
			+	0.000000000
20	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
1025	0.163133800	+ - 0.006266567	2	0.045472838
			+	0.034374234
21	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
701	0.111567620	+ - 0.004896759	4	0.090945661
			+	0.051561343
22	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
525	0.083556294	+ - 0.004097465	0	0.000000000
			+	0.000000000
23	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
416	0.066208422	+ - 0.003567796	3	0.068209231
			+	0.043395327
24	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
312	0.049656343	+ - 0.003022570	1	0.022736419
			+	0.023534430
25	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
283	0.045040850	+ - 0.002860562	1	0.022736419
			+	0.023534430
26	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
226	0.035969015	+ - 0.002524189	1	0.022736419
			+	0.023534430
27	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
226	0.035969015	+ - 0.002524189	0	0.000000000
			+	0.000000000
28	0	0.000000000	0	0.000000000
	0	0.000000000	0	0.000000000
356	0.056659047	+ - 0.003259244	0	0.000000000
			+	0.000000000

ANGULAR DISTRIBUTION OF RELATIVE PARTICLE IMPACT DENSITY AROUND OUTER CONICAL SURFACE OF ELEMENTS

## PRIMARY PARTICLES

## SPUTTERED PARTICLES

ANGULAR DISTRIBUTION OF PARTICLES AROUND OUTER CONICAL SURFACE OF ELEMENTS

## PRIMARY PARTICLES

## SPUTTERED PARTICLES

TABLE OF INCIDENCE ENERGY OF PRIMARY PARTICLES ON SURFACES

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

TABLE OF INCIDENCE ENERGY OF PRIMARY PARTICLES ON SURFACES

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

**TABLE OF INCIDENCE ENERGY OF PRIMARY PARTICLES ON SURFACES**

INSIDE OF OUTER ELEMENTS														
10%		20%		ENERGIES AS PERCENTAGE OF INPUT ENERGY OF				1000.000EV			80%		90%	
				30%	40%	50%	60%	70%	80%	90%	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1	0	1	0	1	0	0	1	0	1	0	0	0
1	2	0	2	0	0	1	0	1	0	0	1	0	0	0
3	1	0	1	0	0	1	2	0	0	1	3	0	0	1
1	1	1	1	0	0	0	1	0	1	0	0	0	1	0
1	0	1	1	0	0	1	0	2	0	0	1	0	2	1
2	1	3	0	2	1	0	4	0	1	0	1	0	6	2
2	3	1	1	2	0	0	1	0	2	4	2	2	0	1
7	8	1	3	1	4	3	0	4	0	5	1	1	0	2
6	2	6	3	2	4	1	4	1	2	0	1	4	3	4
1	3	3	2	3	0	1	1	3	1	2	0	2	5	1
4	3	1	4	1	3	2	3	1	2	2	1	1	4	1
1	3	6	3	2	1	1	2	0	1	2	1	0	3	0
2	2	3	0	0	0	0	2	0	2	2	3	0	2	0
0	0	0	2	0	1	1	3	1	0	1	2	1	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	10	19	12	14	12	18	11	6	17	12	14	16	15	11
20	18	16	12	7	14	12	11	14	8	15	8	13	11	14
25	11	17	17	14	12	7	11	11	15	11	9	23	12	13
22	23	14	11	17	11	6	10	12	6	10	12	12	16	10
25	15	11	8	8	6	6	12	8	12	7	6	14	9	11
26	17	9	14	9	8	8	5	6	10	11	7	13	8	10
22	23	16	7	12	8	10	4	8	6	7	4	9	6	7
26	19	14	8	12	8	7	6	8	12	8	5	7	7	5
23	16	8	8	10	11	7	10	10	6	5	3	13	6	16
233	180	153	118	119	104	93	103	96	104	106	80	134	111	115
233	180	153	118	119	104	93	103	96	104	106	80	134	111	115
233	180	153	118	119	104	93	103	96	104	106	80	134	111	115

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

TABLE OF INCIDENCE ENERGY OF SPUTTERED PARTICLES ON SURFACES

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

TABLE OF INCIDENCE ENERGY OF SPUTTERED PARTICLES ON SURFACES

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

**TABLE OF INCIDENCE ENERGY OF SPUTTERED PARTICLES ON SURFACES**

LAST LINE SHOWS TOTAL NO. OF PARTICLES PER BIN

MAXIMUM NUMBER OF ENTRIES USED IN TABLE FOR SPUTTERING = 2

AVERAGE CALCULATION TIME PER PRIMARY PARTICLE HISTORY 0.4157320 SECONDS

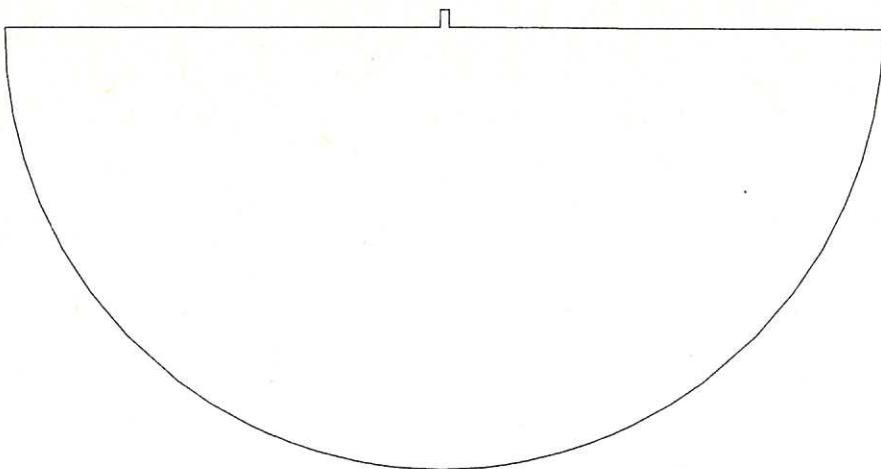
TOTAL TIME USED BY CALCULATION 831.464 SECONDS  
\*\* CYLINDRICAL POCKET - RATIO L/D=2/1 - H+ ON Mo AT 1KEV \*\*

SCALE IS 0.06350 CM PER LENGTH UNIT

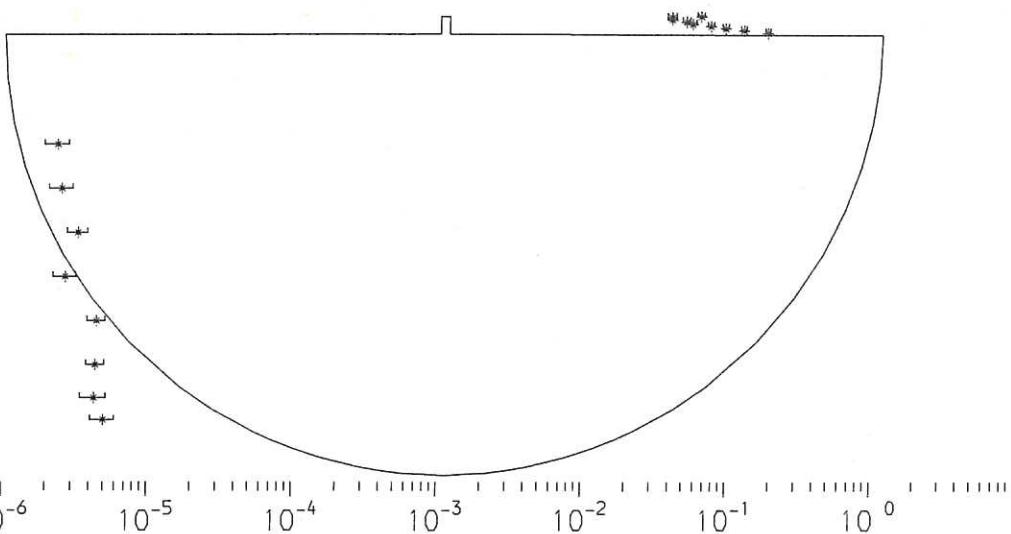
LOG SCALE OF GRAPH PLOTTED VALUES OF DHNAO(I,21) EXTENDS FROM ~6 TO 0

GRAPHICAL OUTPUT COMPLETED

JNCMCO:KEITH .DSET99(S1010\*) PRINTED TO LP1 ON 28/04/78 AT 09:09:42



\*\* CYLINDRICAL POCKET - RATIO L/D=2/1  
- H<sub>+</sub> ON MO AT 1KEV \*\* case number 1011



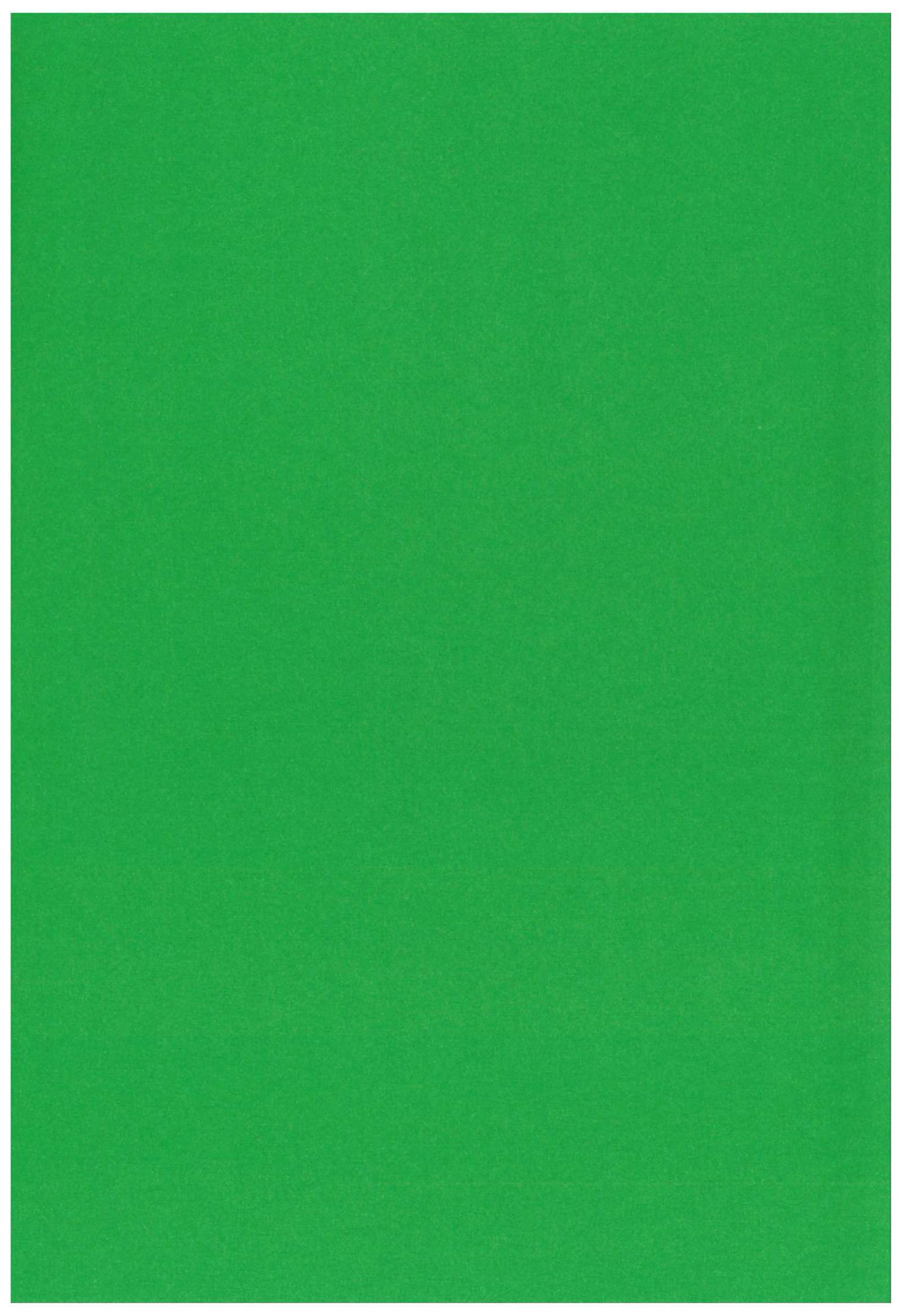
\* interaction probability per unit area at outer surface

○ interaction probability at inner surface

scale 1cm = 0.063499987

\*\* CYLINDRICAL POCKET - RATIO L/D=2/1  
- H<sub>+</sub> ON MO AT 1KEV \*\* case number 1011





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