

**MAX-PLANCK-INSTITUT                    FÜR PLASMAPHYSIK**  
**GARCHING BEI MÜNCHEN**

■ SPUTTERING STUDIES WITH THE  
MONTE-CARLO PROGRAM TRIM SP

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IPP 9/41

August 1983

*Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem  
Max-Planck-Institut für Plasmaphysik und der Europäischen Atomgemeinschaft über die  
Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.*

Abstract

This report shows the results of an thorough investigation about the ability of the Monte-Carlo Program TRIM SP to give data on sputtering. The results show the importance of different processes leading to sputtering, they are compared with predictions of transport theory /1/, they are compared with experimental data and they give details of angular and energy distributions of sputtered particles. Many of the calculated data are given in two papers /2, 3/. The program is described in /2/.

Input parameters

Input parameters to the program are the following:

$Z_1, M_1$  charge and mass of the incident particle

$Z_2, M_2$  charge and mass of the target atom

$p$  density of the target material

$E_q$  energy of the incident particle

$\alpha$  angle of incidence

$E_B$  binding energy of an atom in the bulk  
(always taken as zero if not stated otherwise)

$E_s$  surface binding energy of a target atom at  
the surface(heat of sublimation) from /4/

interaction potential (Kr-C potential /5/ for all collisions  
if not stated otherwise

inelastic energy loss (equipartition of Lindhard-Scharff /6/  
and Oen-Robinson /7/ for all particles  
heavier than He, and Andersen-Ziegler /8/ for  
H, and Ziegler /8/ for He, if not stated  
otherwise) .

All these input parameters are taken from tables and publications and no fitting to experimental data has been done.

For the calculation of the data the TRIM sputtering version TRSPCR1 was used. This version neglects additional scattering with more distant atoms especially at low energy and underestimates surface scattering. This leads to sputtering yields which are larger (30 % for Ne + Ni, 5% for H -> Ni) than those calculated with the new corrected version TRSP1C (see the discussion in /2/). Other small deviations arise in the angular distributions at grazing exit angles and for heavy particles at low energies.

Calculated data

$Y$ , total sputtering yield

$Y_s$ , sputtered energy

Number of sputtered particles for four sputtering processes

- 1) Ion in, PKA;
- 2) Ion in, SKA;
- 3) Ion out, PKA and
- 4) Ion out, SKA.

Number of sputtered particles (all sputtered particles and PKA's alone) versus the energy,  $E$ , of the sputtered particles and the polar exit angle,  $\beta$ , in form of a matrix.

Number of sputtered particles (all sputtered particles and PKA's alone) versus the polar exit angle,  $\beta$ , and the azimuthal exit angle,  $\phi$  (=  $y$ ?), in form of a matrix.

Number of sputtered particles versus the exit energy,  $E$ , and the polar exit angle,  $\beta$ , in an azimuthal exit-angle range,  $A\phi = 15^\circ$ , again in form of a matrix.

Number of sputtered particles (all sputtered particles and PKA's alone) versus the exit energy,  $E$ , and the depth of origin, in form of a matrix.

In addition the program gives some data on reflection:

Particle ( $R_p$  and energy ( $R_E$ ) reflection coefficients.

Number of backscattered particles versus the exit angle,  $E$ , and the polar exit-angle,  $\beta$ , in form of a matrix. Number of backscattered particles versus the azimuthal exit angle,  $\phi$  (=  $y$ ?), and the polar exit-angle,  $\beta$ , in form of a matrix.

The program gives also some data on particle and energy deposition in the solid:

Depth distribution of implanted particles and the first four moments.

Total pathlength distribution of implanted particles.

Depth distribution of energy lost in elastic as well as in inelastic collisions.

The energy resolution is in most cases 1 eV, the angular resolution in  $\beta$  as well as  $\delta$  is  $3^\circ$ . The depth resolution for the depth or origin of the sputtered particles is given in  $\delta$ , the resolution for the depth distribution of implanted particles larger or equal than 18, depending on the maximum penetration depth.

Further calculated data and comparisons with experimental data are given in /11-16/.

### Results

Here only a collection of the calculated sputtering data are given. For a discussion of the results see /2/ and /17/.

Fig. 1 Range of target atoms

Fig. 2-3 Sputtering yield versus incident energy: dependence on interaction potential and inelastic energy loss.

Fig. 4-17 Contribution of different processes to the sputtering yield for several incident ions on Ni: dependence on incident energy and angle.

Fig. 18 Dependence of the sputtering yield on the surface binding energy.

Fig. 19 Dependence of the sputtering yield on the bulk binding energy.

Fig. 20-21 Comparison of the sputtering yield versus incident energy and angle with experimental data.

Fig. 22-23 Total angular distributions for normal and non-normal incidence.

Fig. 24-27 Angular distributions in the incident plane for non-normal incidence.

Fig. 23-32 Contour line plots of the angular distributions for non-normal incidence

Fig. 33 Comparison of the angular distribution for a planar and a scalar surface potential.

Fig. 34-43 Theoretical curves for the sputtering in one binary collision for a planar and a scalar potential.

Fig. 44-47 Comparison of the computer simulation results with the analytical formulae for the sputtering in one binary collision: Angular distributions.

Fig. 48-51 Total energy distributions for non-normal incidence.

Fig. 52-55 Energy distributions in different emission directions for non-normal incidence.

Fig. 56-58 Comparison of computer simulation results with the analytical formulae for the sputtering in one binary collision: Energy distributions.

Fig. 59 Escape depth of sputtered particles.

Fig. 60-61 Definition of angles.

Sputtering in one binary collision /"17/

a) Angular distributions

The occurrence of the ridge in the angular distribution is shown to be due to PKA in fig. 28. In addition it can be demonstrated that the ridge is mainly due to sputtering in one binary collision. From fig. 61 the polar exit angle  $\beta$  after refraction (planar surface potential) is found to be

$$\operatorname{tg}^2 \beta = \frac{E_H}{E_x} \quad (1)$$

with

$$E_H = T \sin^2 \beta'$$

$$E_x = T \cos^2 \beta' - E_0$$

where  $T$  is the transferred energy in a binary collision and  $\beta'$  is the emission angle before refraction.

The transferred energy is

$$T = Y E_0 \cos^2 \theta_r$$

where

$$Y = \frac{4M_1 M_2}{(m_1 + m_2)^2}$$

The recoil angle  $\phi_r$  can be determined from fig. 60

$$\cos \phi_r = \sin a \sin \beta' \cos \theta_r - \cos a \cos \beta' \quad (2)$$

From these relations the polar exit angle  $\beta$  is calculated by

$$\tan^2 \beta = \frac{A[\sin a \sin \beta' \cos \theta_r - \cos a \cos \beta']^2 \sin^2 \beta'}{A[\sin a \sin \beta' \cos \theta_r - \cos a \cos \beta']^2 \cos^2 \beta' - 1} \quad (3)$$

with  $A = Y E_0 / E_S$ ,

Due to the limitation of  $\beta'$  caused by a maximum recoil angle,  $\phi_R = 90^\circ$ ,  $\beta$  must have a minimum value,  $\beta_{\min}$ . Differentiation leads to the following transzental equation for  $\beta'_{\min}$

$$A = \frac{\sin a \sin 2\beta'_{mm} \cos \langle f \rangle - \cos a \cos 2\beta'_{mm}}{(\sin a \sin \beta'_{min} \cos \langle J \rangle - \cos a \cos \beta'_{min}) \cos \beta'_{mm}} \quad (4)$$

Putting  $\beta_{in}$  into equation (3) gives  $\beta_{min}$ . An example of  $\beta$  versus  $\beta'$  is shown in fig. 34. The assumption is made that the angle  $\beta_{min}$  occurs with the highest intensity for a binary collision sputtering process, which is justified by taking the cross section into account /17/.

As seen from fig. 34,  $\beta'$  has a lower and an upper limit,  $\beta_{min}$  and  $\beta_{max}$ . They can be calculated from equation (3) by putting the denominator in (3) to zero. The result is

$$\cos^2 \beta_{1,2} = \frac{-[2B \cos a - \sin^2 a \cos \langle J \rangle + \sin a \cos \langle J \rangle (\sin^2 a \cos i)] - 4B(B + \cos a)}{27(\cos^2 a + \sin^2 a \cos^2 J)} \quad (5)$$

with  $B = A^{-1/2}$

Figure 35 shows  $\beta_{min}$ ,  $\beta'_{min}$ ,  $\beta'_1$  and  $\beta'_2$  versus the azimuthal angle,  $\alpha$ , for a chosen value of  $A$ . The next figures 36-33 show  $\beta_{mm}$  versus  $\alpha$ ,  $a$  and  $A$ .

There is an upper limit for the azimuthal angle which is determined from (5) by putting the square root to zero:

$$\cos^2 \alpha_c = \frac{4B(B + \cos a)}{\sin^2 a} \quad (6)$$

There is also a lower limit for  $a$  and  $A$  which follows from  $\alpha_c = 0$ :

$$\cos a_c = 1 - 2B \quad \text{or} \quad A_c = [\sin \alpha]^4 \quad (7)$$

The critical value,  $\alpha_c$ , is shown in fig. 39, 40 versus  $a$  and  $A$ , the relation between  $a_c$  and  $A$  in fig. 41.

If one assumes a scalar potential (no refraction) there is also a lower limit for the exit angle: starting from

$$E_S = T = Y_E O \cos^2 R \quad (8)$$

the exit angle  $\beta_{\min}$  in this case is determined by (8) and (2)

$$\cos \beta_{\min} = \frac{-B \cos a + \sin \cos \phi [\cos^2 a + \sin^2 a \cos^2 \phi - B^2]^{1/2}}{\cos^2 a + \sin^2 a \cos^2 \phi} \quad (9)$$

The lower limit of  $\beta_{\min}$ ,  $\beta$ , is determined for  $\alpha = 90^\circ$  or  $B = 0$

$$\cos \beta = \frac{\sin a \cos \phi}{[\cos^2 a + \sin^2 a \cos^2 \phi]^{1/2}} \quad (10)$$

Again, as above, for the planar potential the upper limit for  $\phi$ ,  $\phi_c$ , is determined by  $\beta_{\max} = 90^\circ$  in (9) with the result

$$\frac{4}{c} = - ? - \frac{\sin a}{\cos a} \quad (11)$$

and the lower limit for  $a$ ,  $a_c$ , is found by  $\frac{4}{c} = 0$

$$\sin a_c = A^{-1/2} = B \quad (12)$$

Curves for  $\beta_{\min}$ ,  $\phi_c$ ,  $a_c$  determined for several values of  $A$  are shown in fig. 42, 43.

### b) Energy distributions.

The second peak in the energy distributions in the forward direction can be related to the sputtering in one binary collision.

The energy,  $E$ , a particle has after sputtered in a binary collision is

$$E = T - E_0$$

The emission angle,  $\beta$ , after refraction is given by taking (1) into account.

$$\operatorname{tg}^2 \beta = \frac{(E' + 1) \sin^2 \beta}{(E' + 1) \cos^2 \beta - 1} \quad (13)$$

where  $E' = \frac{\epsilon}{\epsilon_s}$ .

The relation between  $\beta$  and  $E$  is determined by calculating  $\beta'$  from

$$\cos \beta' = \frac{-\sqrt{E'^2 + 1} \cos a' \sin a \cos \theta / \cos^2 a + \sin^2 a \cos^2 \theta - E'^2 - 1}{\cos^2 \theta + \sin^2 a \cos^2 \theta} \quad (14)$$

The curve resulting from (13) and (14) is shown for some examples in figs. 56-58.

For the case of a scalar surface potential, the relation between  $E$  and  $\beta$  is

$$\begin{aligned} E &= E_0 [A \cos^2 \theta_K - 1] \\ &= E_0 [A (\sin a \sin \beta \cos \theta - \cos a \cos \beta)^2 - 1] \end{aligned} \quad (15)$$

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### Figure Captions

Fig. 1 Sputtered particles per incident particle versus the depth,  $x_q$ , of the starting particle for 100 eV Ni in Ni.

The fraction of escaping starting particles are given for two different inelastic energy losses:  
LS (+) and OR (x).

The fraction of sputtered SKA are given for the same two inelastic energy loss models:  
LS (o) and OR (•).

Indicated in the figure is also the range parameter R (and 2 R) applied in TRIM to reduce computer time.

The Kr-C potential was applied for the calculations.

Fig. 2 Ne bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .  
Sputtering yield, Y, versus the incident energy, E, for different interatomic potentials and inelastic energy loss models. Comparison with experimental data (o)/9/.  
a) Molière potential for Ne-Ni, Kr-C potential for Ni-Ni (solid lines). Molière potential for both kinds of collisions (dashed lines).  
b) Kr-C potential for both Ne-Ni and Ni-Ni collisions.  
Lines drawn to guide the eye.

Fig. 3 H bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .  
Sputtering yield, Y, versus the incident energy, E, for different interatomic potentials and inelastic energy loss models.  
a) Molière potential for H-Ni, Kr-C potential for Ni-Ni.  
b) Kr-C potential for both kinds of collisions.  
Lines drawn to guide the eye.

Fig. 4 H bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R$ , versus the incident energy,  $E_q$ .
- b) Relative contribution of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig. 5 D bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R$ , versus the incident energy,  $E_q$ .
- b) Relative contribution of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig. 6 T bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R$ , versus the incident energy,  $E_q$ .
- b) Relative contribution of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig. 7 He bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R$ , versus the incident energy,  $E_q$ .
- b) Relative contribution of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig. 8 Comparison of the sputtering yield,  $Y$ , of Ni with T and He versus the incident energy,  $E_q$ , for normal incidence,  $\alpha = 0^\circ$ .

Lines drawn to guide the eye.

Fig. 9  $^4\text{He}$  bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_j$ , versus the incident energy,  $E$ .
- b) Relative contribution of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig. 10 Ne bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R$ , versus the incident energy,  $E_q$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the incident energy,  $E$ .  
Lines drawn to guide the eye.

Fig. 11 Ar bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_j$ , versus the incident energy,  $E_q$ . In addition, the sputtering yield is shown as calculated from Sigmund's theory, using  $F_d(x=0) = c \cdot e \cdot S_n(E_0)$  for both the Moliere and the Kr-C potential.
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out) and secondary knock-on atoms, SKA (ion in and ion out) to the total sputtering yield,  $Y$  versus the incident energy  $E$ .  
Lines drawn to guide the eye.

Fig.12 Xe bombardment of Ni at normal incidence,  $\alpha = 0^\circ$ .

- a) Sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out) to the total sputtering yield,  $Y$ , versus the incident energy,  $E_q$ .  
Lines drawn to guide the eye.

Fig.13 H bombardment of Ni at an incident energy  $E_q = 1$  keV:

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_j$ , versus the angle of incidence,  $\alpha$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ .

Lines drawn to guide the eye.

Fig.14  $^4\text{He}$  bombardment of Ni at an incident energy,  $E_q = 1$  keV

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_n$ , versus the angle of incidence,  $\alpha$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ .

Lines drawn to guide the eye.

Fig.15 Ne bombardment of Ni at an incident energy  $E_q = 1$  keV:

- a) Sputtering yield,  $Y$ , for three different inelastic energy loss models, and particle reflection coefficient,  $R_{\text{in}}$ , versus angle of incidence,  $\alpha$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ .

Lines drawn to guide the eye.

Fig.16 Ar bombardment of Ni at an incident energy,  $E_q = 1$  keV:

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_j$ , versus the angle of incidence,  $\alpha$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ .

Lines drawn to guide the eye.

Fig.17 Xe-bombardment of Ni at an incident energy  $E_q = 1$  keV:

- a) Sputtering yield,  $Y$ , and particle reflection coefficient,  $R_j$ , versus the angle of incidence,  $\alpha$ .
- b) Relative contributions of primary knock-on atoms, PKA (ion in and ion out), and secondary knock-on atoms, SKA (ion in and ion out), to the total sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ .

Fig.18 a) Sputtering yield,  $Y$ , versus surface binding energy,  $E_s$ , for 1 keV Ar on Ni at normal incidence. The dashed line gives  $Y = E_s^{-1}$ .

b) Sputtering yield,  $Y$ , versus surface binding energy,  $E_s$ , for 0.08, 0.3 and 2 keV D on C at normal incidence.  
The dashed line gives  $Y \propto E_s^{-1}$ .

Fig.19 Sputtering yield,  $Y$ , versus the normalized ion energy,  $E'$ , where  $E' = E/E_{th}$  with  $E_{th}$  defined in /10/ for D on Ni at normal incidence. The curves show the influence of various choices of bulk binding energies. The curve is determined from the semi-empirical formula (7) from Ref. /10/.

Fig.20 Comparison of experimental /9,1c) / and calculated values of the sputtering yield,  $Y$ , versus incident energy,  $E_q^4$ , for H, D, He, Ne, Ar and Xe on Ni at normal incidence.

Lines connect the calculated points and are drawn to guide the eye .

Fig.21 Comparison of experimental /10/and calculated values of the sputtering yield,  $Y$ , versus the angle of incidence,  $\alpha$ , for H on Ni.

- a) incident energies from 0.2 keV to 1 keV.
- b) incident energies from 4 keV and to 8 keV.

Fig.22 Angular distribution of sputtered particles for 1 keV H bombardment of Ni at normal incidence. The polar angle distribution is azimuthally symmetric. The total angular distribution (solid line), a cosine distribution (circle) and the contribution of primary knock-ons (dashed line) are shown.

Fig.23 Azimuthal distribution (integrated over polar angles) of sputtered particles for 1 keV H bombardment of Ni at an angle of incidence,  $\alpha = 80^\circ$ .

Fig.24 Angular distributions in the incident plane of the sputtered particles (azimuthal angular range  $0^\circ < \theta < 15^\circ$ ) for 1 keV H bombardment of Ni at several angles of incidence. The distributions are normalized to give the same maximum value.

Fig.25 Angular distributions of sputtered particles in the incident plane (azimuthal angular range  $0^\circ < \theta < 15^\circ$ ) for H bombardment of Ni at an angle of incidence,  $\alpha = 80^\circ$ , and for several incident energies  $E_i$ . The distributions are normalized to give the same maximum value .

- Fig. 26 Angular distributions of sputtered particles in the incident plane (azimuthal angular range  $0^\circ < \langle j \rangle < 15^\circ$ ) for the bombardment of Ni with different incident particles with an incident energy,  $E_q = 1$  keV, and an angle of incidence,  $\alpha = 80^\circ$ . The distributions are normalized to give the same maximum value.
- Fig. 27 Angular distribution of sputtered particles in the incident plane (azimuthal angular range  $0 < \langle j \rangle < 15^\circ$ ) for D bombardment of Ni, Mo and W with an incident energy,  $E_q = 4$  keV, and an angle of incidence,  $\alpha = 80^\circ$ . The distributions are normalized to give the same maximum value.
- Fig. 28 Contour plots (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for D bombardment of Ni at an incident energy of 4 keV and an angle of incidence of  $\alpha = 80^\circ$ .
- angular distribution of all sputtered particles
  - angular distribution of primary knock-on atoms (PKA)
  - angular distribution of secondary knock-on atoms (SKA)
- Fig. 29 Contourplot (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for D bombardment of Mo at an incident energy of 4 keV and an angle of incidence of  $\alpha = 80^\circ$ .
- Fig. 30 Contourplot (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for D bombardment of W at an incident energy,  $E_q = 4$  keV and an angle of incidence of  $\alpha = 80^\circ$ .

Fig.31 Contour plots (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for Ne bombardment of Ni at an incident energy of 3 keV and an incident angle,  $\alpha = 75^\circ$ .

- a) angular distribution of all sputtered particles
- b) angular distribution of primary knock-on atoms (PKA)
- c) angular distribution of secondary knock-on atoms (SKA).

Fig.32 Contour plots (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for 350 eV D bombardment of C at an incident angle,  $\alpha = 80^\circ$ .

- a) planar potential, surface binding energy,  $E_s = 7.4$  eV
- b) without refraction, (scalar potential) surface binding energy,  $E_s = 7.4$  eV.

Fig.33 Angular distributions of sputtered particles in the incident plane (azimuthal angular range  $0 < \theta < 15^\circ$ ) for 350 eV D bombardment of C at an incident angle,  $\alpha = 80^\circ$ .

- planar potential, surface binding energy,  $E_s = 7.4$  eV
- without refraction, (scalar potential), surface binding energy,  $E_s = 7.4$  eV.

Fig. 34 Polar angle  $\beta$  of sputtered particles (after refraction) versus the starting polar angle  $\beta'$  (in a binary collision) in the incident plane ( $\theta = 0^\circ$ ) calculated by formula (3).

The example is determined for 4 keV D bombardment of Ni at an incident angle,  $\alpha = 80^\circ$ .

- Fig.35 The polar angles  $\beta$ ,  $\beta'$ ,  $\beta_{in}$  versus the azimuthal angle,  $\phi$ , calculated by formula (3,5,10).  
The example is determined for 4 keV D bombardment of Ni at an incident angle,  $a = 80^\circ$ .
- Fig.36 Polar angle,  $\beta_{min}$ , versus the azimuthal angle,  $\phi$ , for several values of  $A = yE/E$  and an incident angle,  $a = 80^\circ$ .
- Fig.37 Polar angle,  $\beta_{min}$ , versus the incident angle,  $a$ , in the incident plane ( $\gamma = 0^\circ$ ) for several values of  $A$ .
- Fig. 38 Polar angle,  $\beta_{min}$ , versus the value  $A$  in the incident plane for several values of the incident angle,  $a$ .
- Fig.39 The critical azimuthal angle,  $\phi_t$ , versus the angle of incidence,  $\alpha$ , for several values of  $A$ .
- Fig.40 The critical azimuthal angle,  $\phi_c$ , versus the value  $A$  for several angles of incidence,  $a$ .
- Fig.41 The critical angle of incidence,  $\alpha_c$  (critical value,  $A_c$ ), versus the value  $A$  (angle of incidence,  $a$ ).
- Fig.42 Polar angle,  $\beta_{min}$ , versus the azimuthal angle,  $\phi$ , for several values of  $A$ . The curves are calculated for an incident angle,  $a = 80^\circ$ , and without refraction.
- Fig.43 Critical azimuthal angle,  $\phi_f$ , and critical angle of incidence,  $\alpha_c$ , versus the value  $A$ .  $\phi_f$  is determined for several angles of incidence,  $a$ .
- Fig.44 Comparison of the polar angle,  $\beta_{min}$ , with the polar angle of maximum intensity in the angular distribution of sputtered particles in the incident plane for several ion target combinations at an angle of incidence,  $a = 80^\circ$ .

- Fig.45 Angular distributions of sputtered particles in the incident plane (azimuthal angular range,  $0^\circ < \theta < 15^\circ$ ) for different ion target combinations but with the same value  $A = yE_q/E_s = 19.7$  and an angle of incidence,  $\alpha = 80^\circ$ . The distributions are normalized to give the same maximum value.
- Fig.46 Contour plots (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for 350 eV D bombardment of C at an incident angle,  $\alpha = 80^\circ$ . Inserted is the line  $B_{\min}$  versus calculated from formula ( ).  
a) planar potential,  $E_g = 7.4$  eV  
b) without refraction (scalar potential)  $E_g = 7.4$  eV.
- Fig.47 Contour plot (lines of equal intensity: sputtered atoms per solid angle) of the angular distribution of sputtered particles for 4 keV D bombardment of Ni at an incident angle,  $\alpha = 80^\circ$ . Inserted in the line  $B_{\min}$  versus  $\phi$  calculated from formula ( ).
- Fig.48 Energy distributions of sputtered particles (particles per eV and incident particle) for 0.35 keV D bombardment of C at an incident angle,  $\alpha = 80^\circ$ .  
Planar potential: all sputtered particles (---), and primary knock-on atoms, PKA (---).  
Scalar potential (without refraction): all sputtered particles (-•-)
- Fig.49 Energy distributions of sputtered particles in several azimuthal directions (integrated over the polar angle,  $\beta$ ). C was bombarded with 0.35 keV D at an incident angle,  $\alpha = 80^\circ$ .
- Fig.50 Energy distribution of sputtered particles for 3 keV Ne bombardment of Ni at an incident angle,  $\alpha = 75^\circ$ . Shown are the energy distributions of all sputtered particles (-) and of the PKA (---).

Fig. 51 Energy distributions of sputtered particles in several azimuthal directions (integrated over the polar angle,  $\beta$ ). Ni was bombarded with 3 keV Ne at an incident angle,  $a = 75^\circ$ .

Fig. 52 Contour plots (lines of equal intensity: sputtered atoms per solid angle and energy interval) of the energy - polar angle distribution of sputtered particles for different azimuthal angle intervals 350 eV D bombardment of C at an incident angle,  $a = 80^\circ$ . c; gives the intensity step between adjacent contour lines.

- a) integrated over the azimuthal angle, \$
- b) azimuthal angular range,  $0^\circ < \alpha < 15^\circ$
- c) "  $15^\circ < \alpha < 30^\circ$
- d) "  $30^\circ < \alpha < 45^\circ$
- e) "  $45^\circ < \alpha < 60^\circ$
- f) "  $60^\circ < \alpha < 75^\circ$
- g) "  $75^\circ < \alpha < 90^\circ$
- h) "  $90^\circ < \alpha < 105^\circ$
- i) "  $105^\circ < \alpha < 120^\circ$
- j) "  $120^\circ < \alpha < 135^\circ$
- k) "  $135^\circ < \alpha < 150^\circ$
- l) "  $150^\circ < \alpha < 165^\circ$
- m) "  $165^\circ < \alpha < 180^\circ$

Fig. 53 Energy distributions of sputtered particles in the incident plane ( $0^\circ < \beta < 15^\circ$ ) in several polar-angle intervals for D bombardment of C. Incident energy,  $E_q = 0.35$  keV; incident angle,  $a = 80^\circ$ .

- a)  $12^\circ < \beta < 15^\circ$  and  $27^\circ < \beta < 30^\circ$
- b)  $42^\circ < \beta < 45^\circ$ ,  $57^\circ < \beta < 60^\circ$  and  $72^\circ < \beta < 75^\circ$ .

Fig. 54 Contour plots (lines of equal intensity: sputtered particles per solid angle and energy interval) of the energy-polar angle distribution of sputtered particles for different azimuthal-angle intervals. 3 keV Ne bombardment of Ni at an incident angle,  $\alpha = 75^\circ$ . c gives the intensity step between adjacent contour lines.

a )	integrated over the azimuthal angle ,
b )	azimuthal angular range, $0^\circ < \theta < 15^\circ$
c )	" $15^\circ < \theta < 30^\circ$
d )	" $30^\circ < \theta < 45^\circ$
e )	" $45^\circ < \theta < 60^\circ$
f )	" $60^\circ < \theta < 75^\circ$
g )	" $75^\circ < \theta < 90^\circ$
h )	" $90^\circ < \theta < 105^\circ$
i )	" $105^\circ < \theta < 120^\circ$
j )	" $120^\circ < \theta < 135^\circ$
k )	" $135^\circ < \theta < 150^\circ$
l )	" $150^\circ < \theta < 165^\circ$
m )	" $165^\circ < \theta < 180^\circ$

Fig. 55 Energy distributions of sputtered particles in the incident plane ( $0^\circ < \theta < 15^\circ$ ) in several polar-angle intervals for Ne bombardment of Ni. Incident energy,  $E_0 = 3$  keV, incident angle,  $\alpha = 75^\circ$ .

- a)  $12^\circ < \beta < 15^\circ$  and  $27^\circ < \beta < 30^\circ$
- b)  $42^\circ < \beta < 45^\circ$ ,  $57^\circ < \beta < 60^\circ$  and  $72^\circ < \beta < 75^\circ$ .

Fig. 56 Exit angle,  $\beta$ , versus the energy,  $E$ , of C sputtered in a binary collision with D. The three curves are due to the simple binary collision, and due to an additional scalar and planar potential.

Fig. 57 Contour plot (lines of equal intensity: sputtered particles per solid angle and energy interval) of the energy-polar angle distribution of sputtered particles in the incident plane ( $0^\circ < \langle t \rangle < 15^\circ$ ) for 350 eV D bombardment of C at an incident angle,  $\alpha = 80^\circ$

- a) planar potential; indicated is the curve for a binary collision, see Fig. 56
- b) scalar potential; indicated is the curve for a binary collision, see Fig. 56

Fig. 58 Contour plot (lines of equal intensity: sputtered particles per solid angle and energy interval) of the energy-polar angle distribution of sputtered particles in the incident plane ( $0^\circ < \langle i \rangle < 15^\circ$ ) for 3 keV Ne bombardment of Ni at an incident angle,  $\alpha = 75^\circ$ . Indicated is the curve due to a binary collision (planar potential).

- Fig. 59 Relative number of sputtered particles versus their depth of origin
- a) H bombardment of Ni at normal incidence for three incident energies,  $E_q = 0.5, 5$  and 50 keV.
  - b) Ar bombardment of Ni at normal incidence and for four incident energies,  $E_q = 0.1, 1, 10$  and 100 keV.

Fig. 60 Definition of angles  $\alpha$ ,  $\beta$ , and  $\delta_R$ .

Fig. 61 Surface refraction due to a planar surface potential.

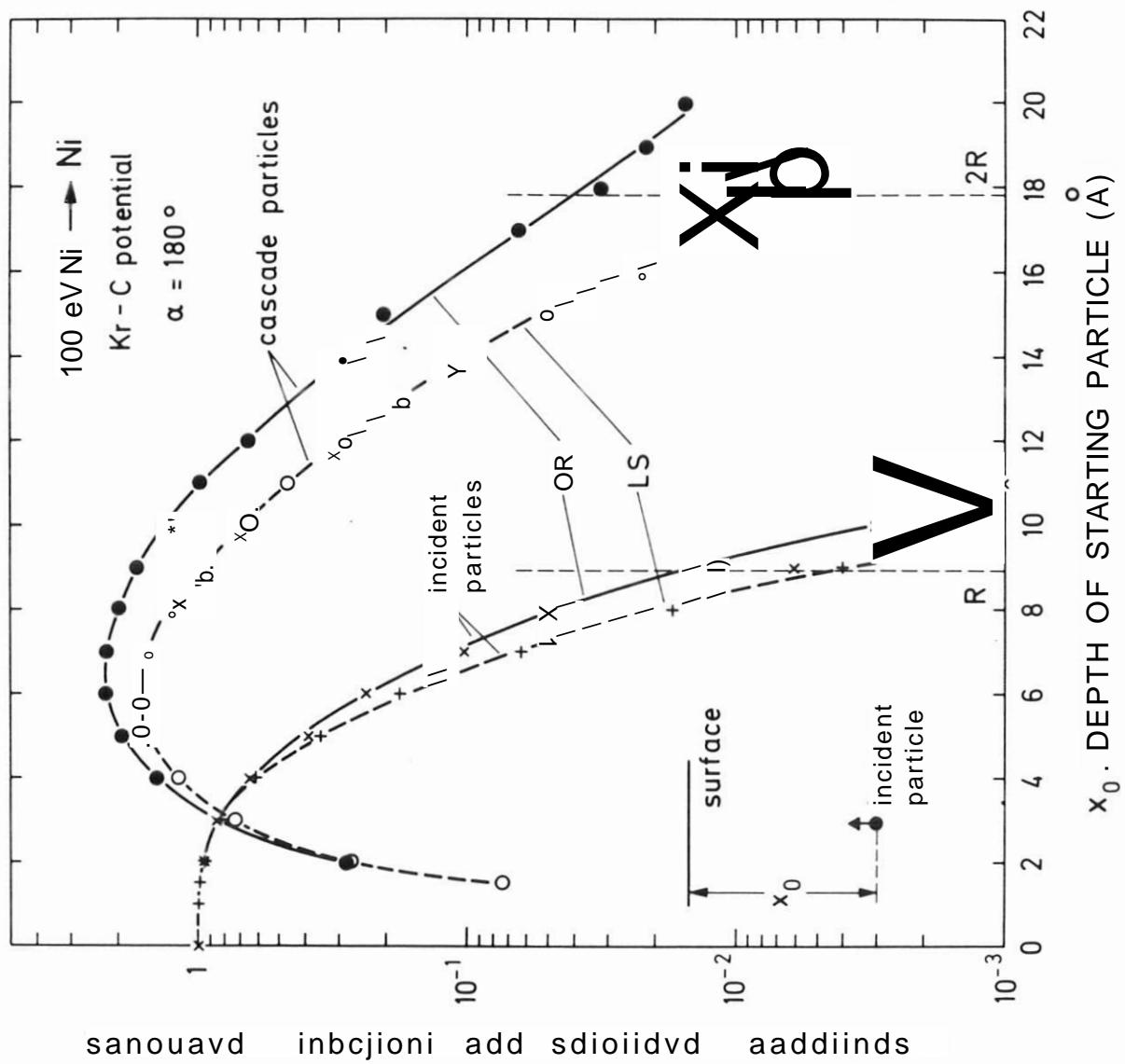


Fig. 1

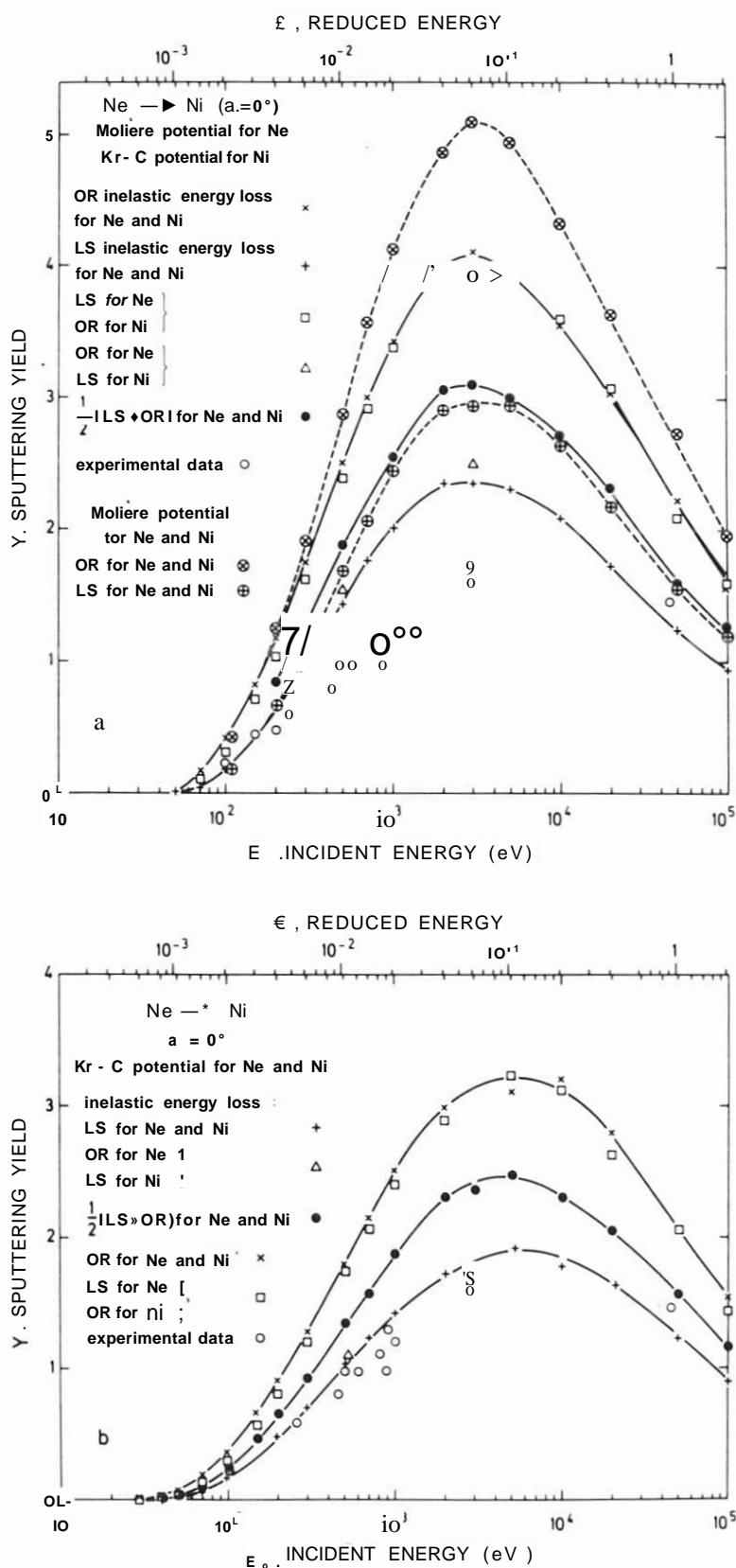


Fig. 2

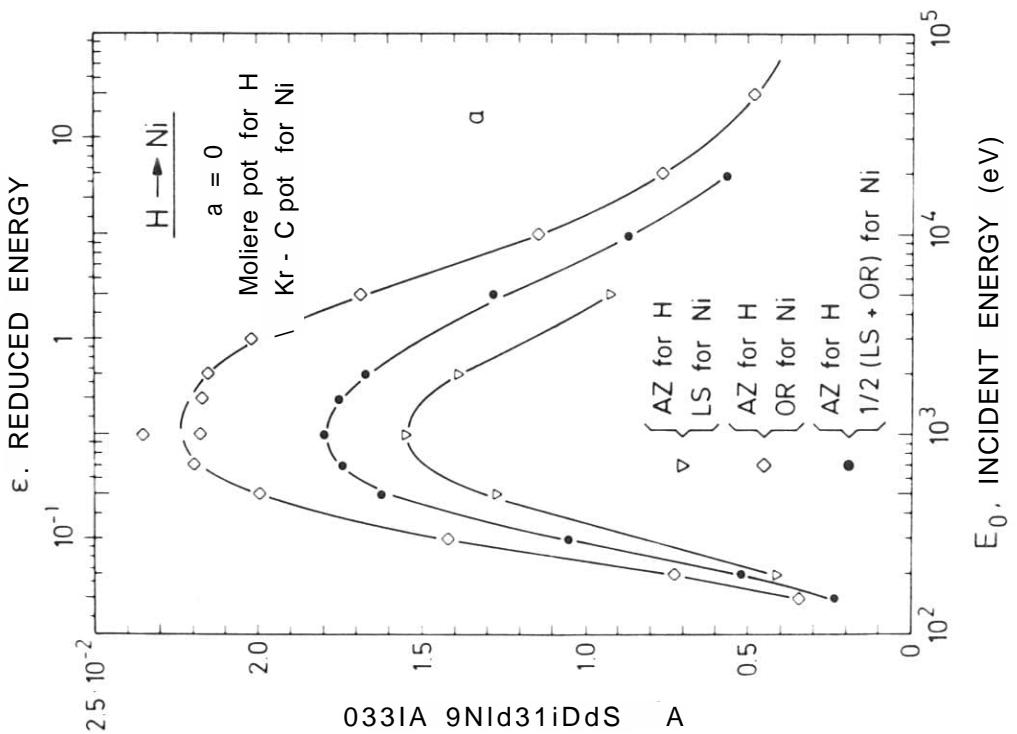
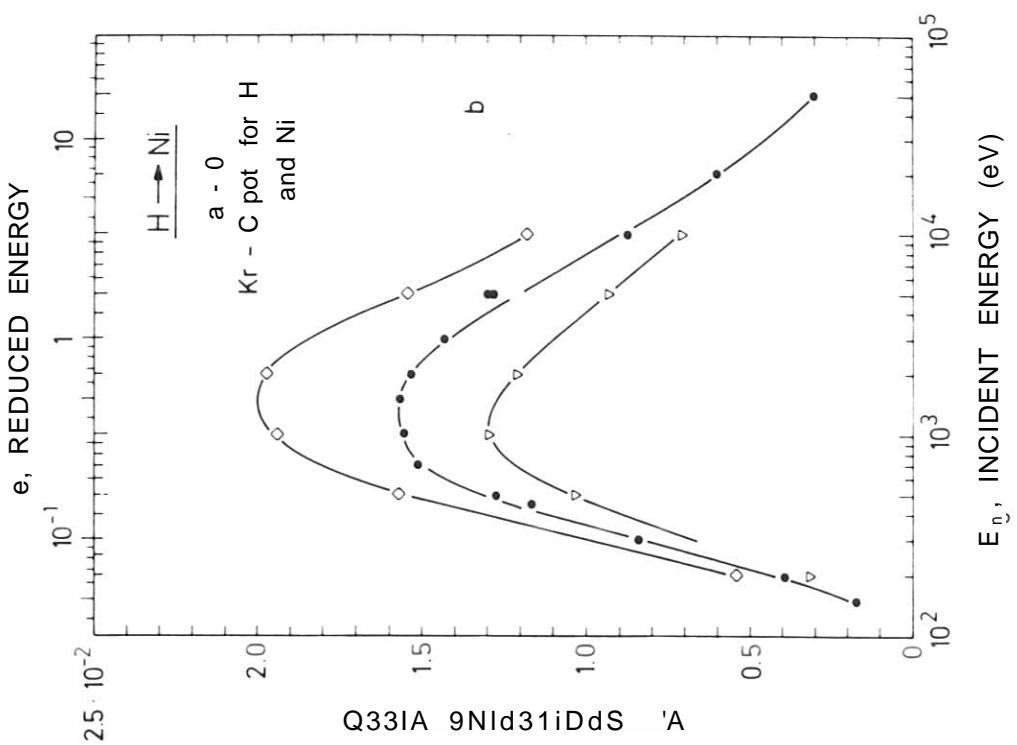


Fig. 3

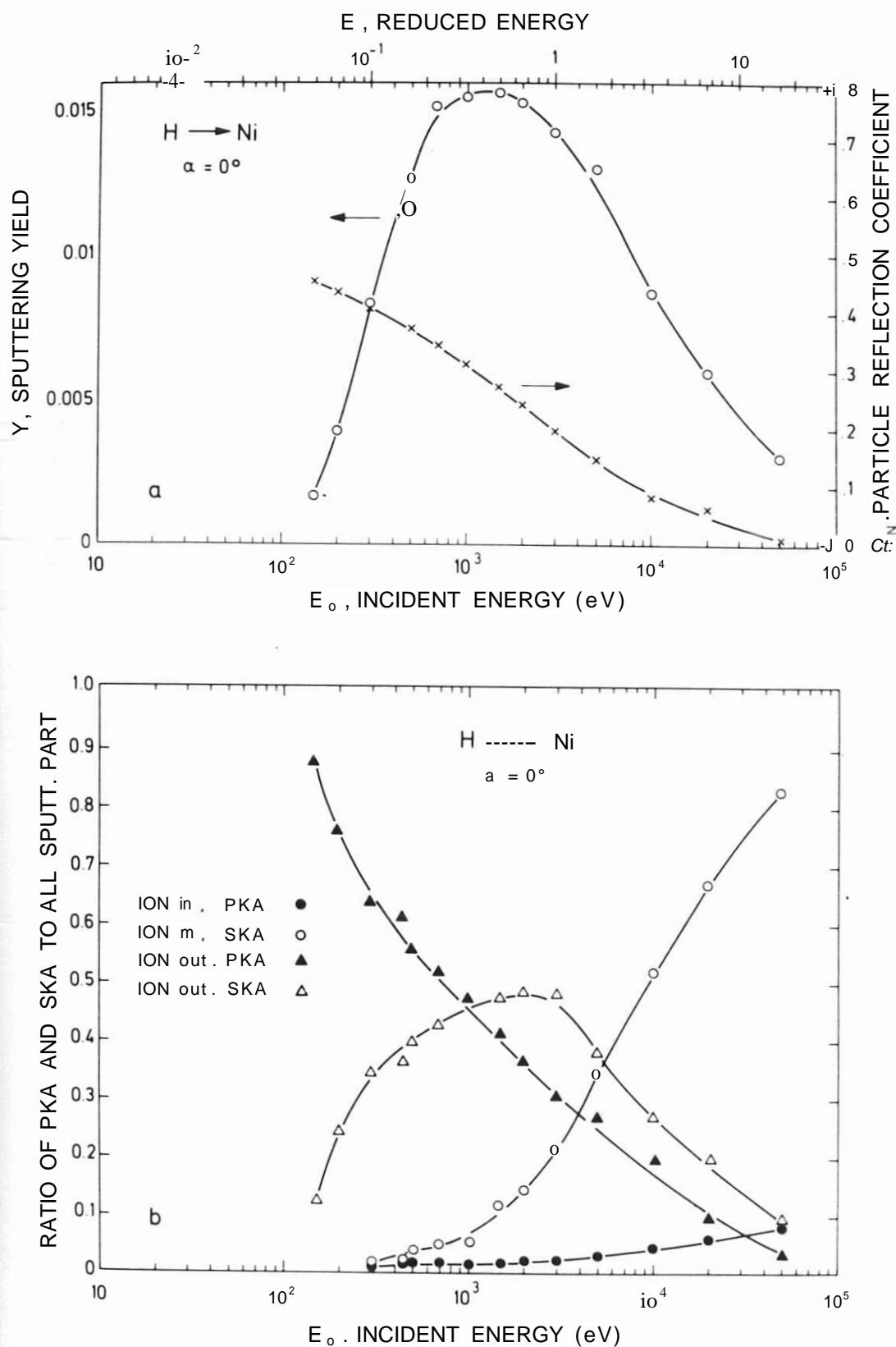


Fig. 4

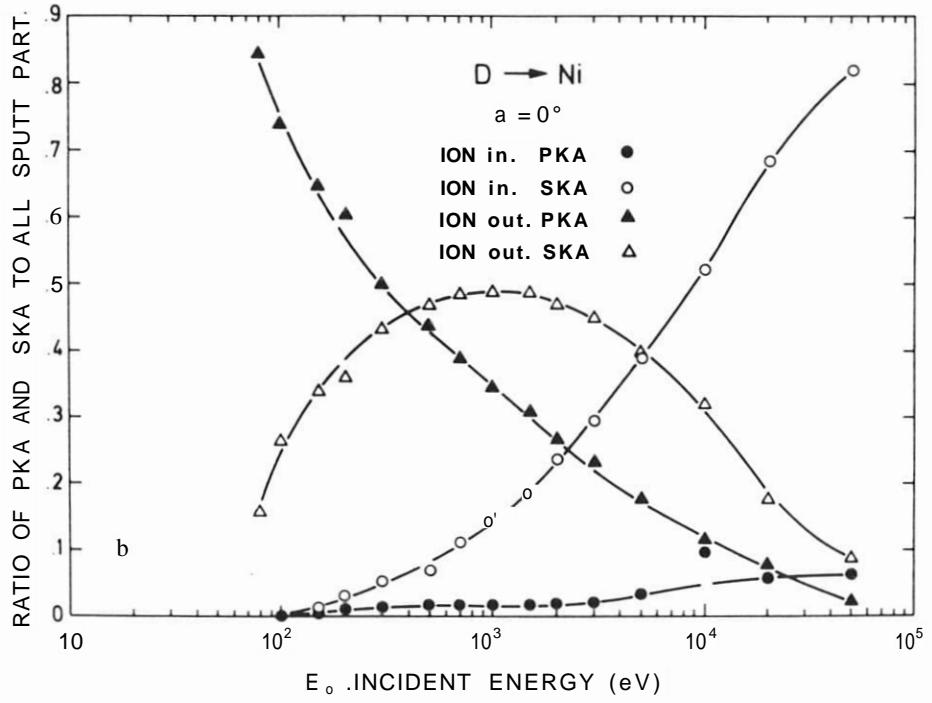
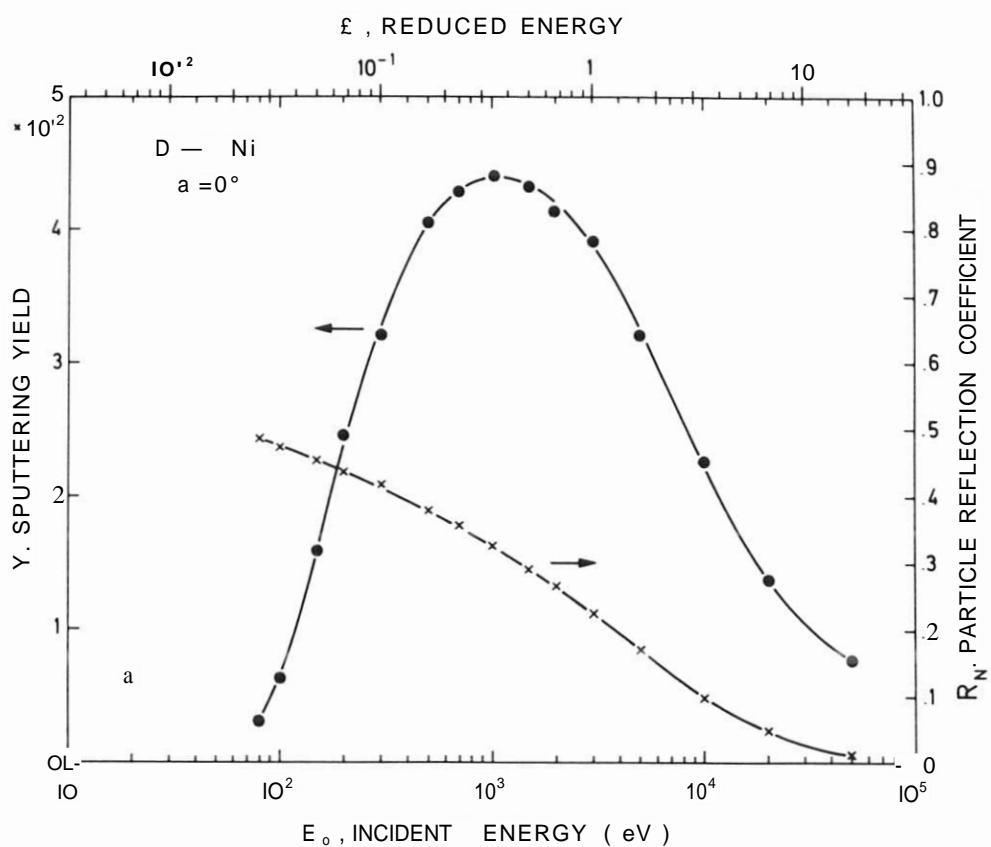


Fig. 5

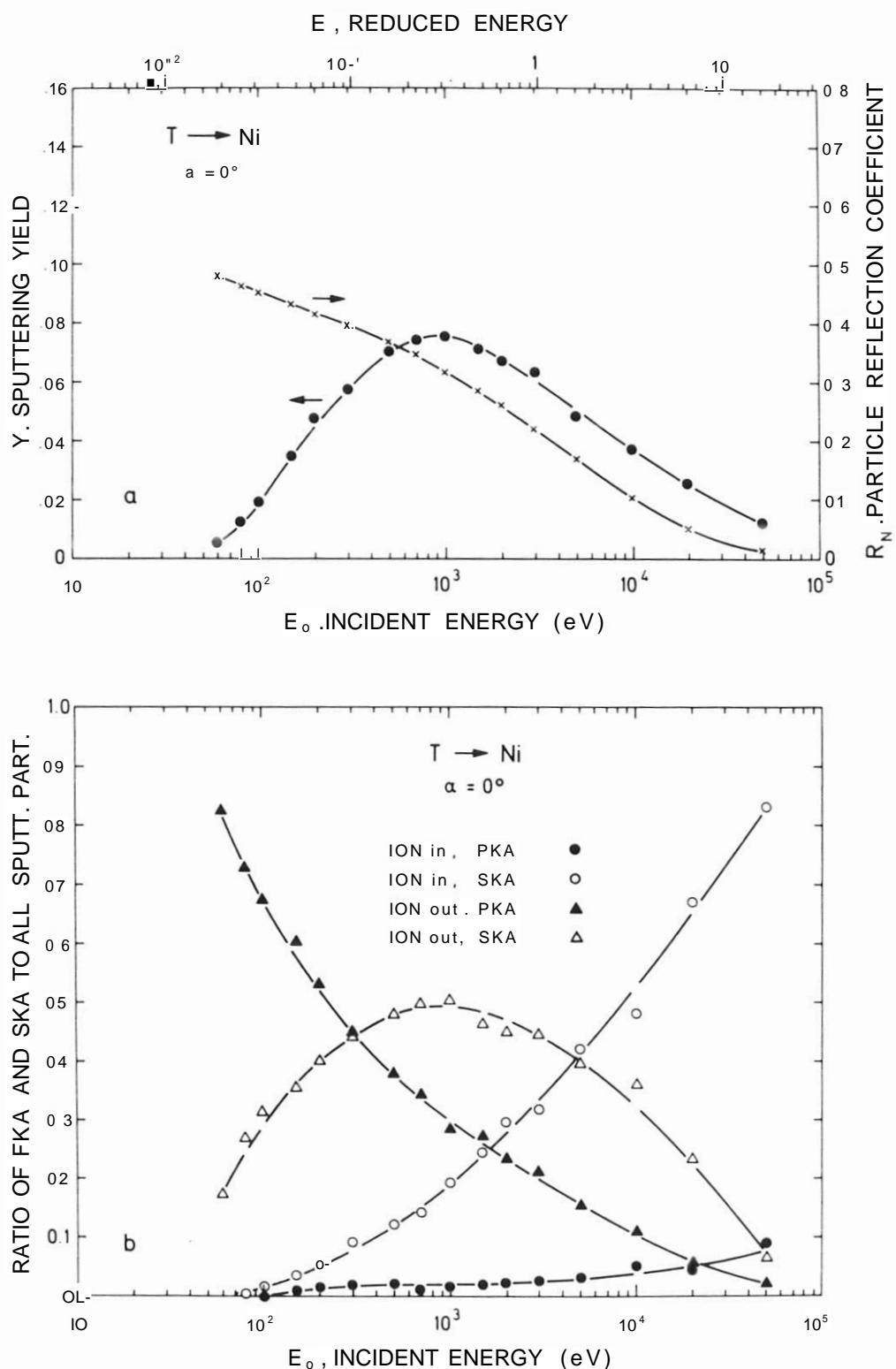


Fig. 6

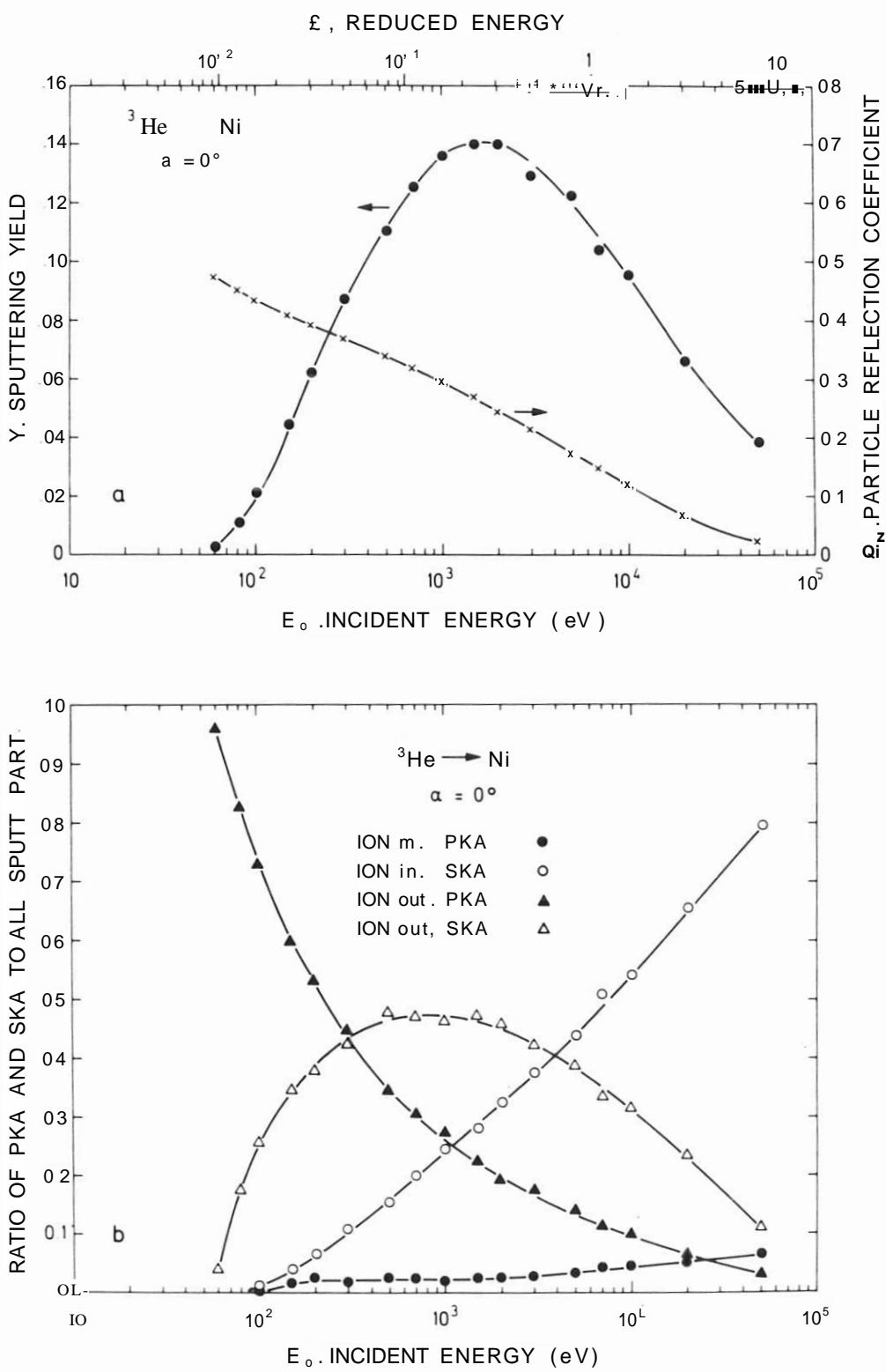


Fig. 7

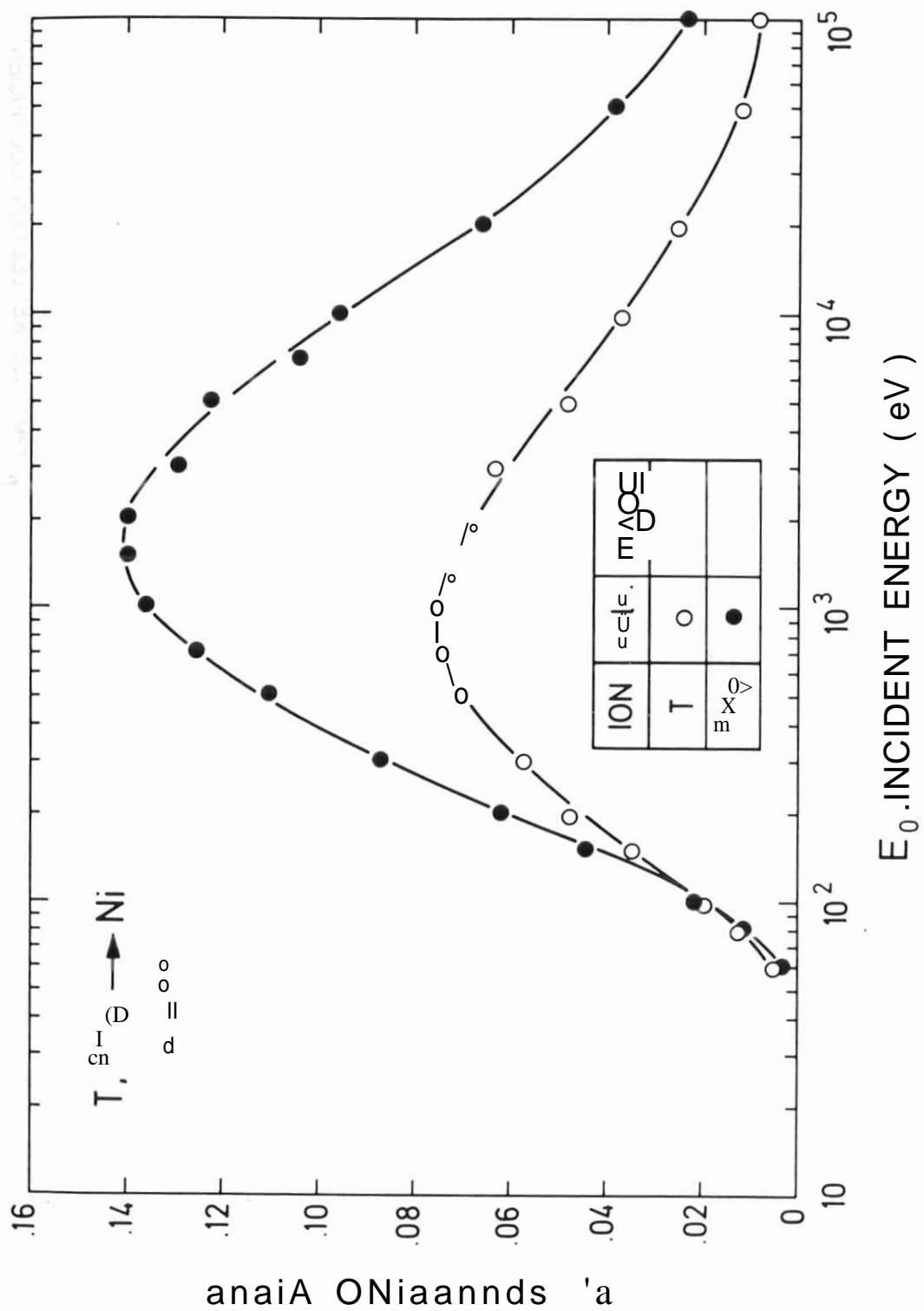


Fig. 8

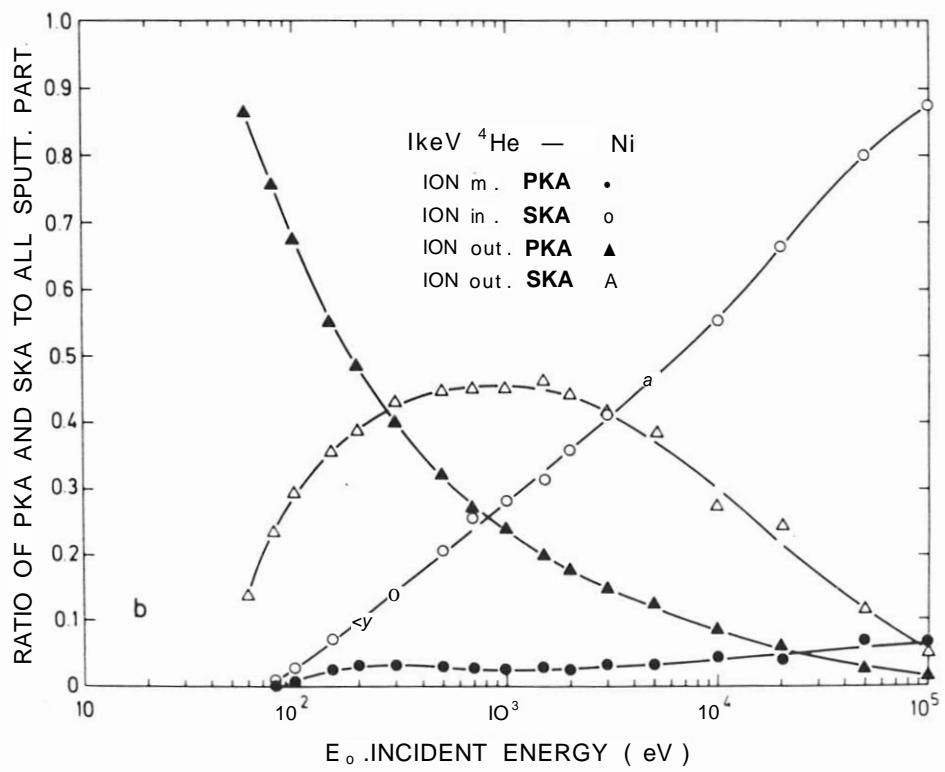
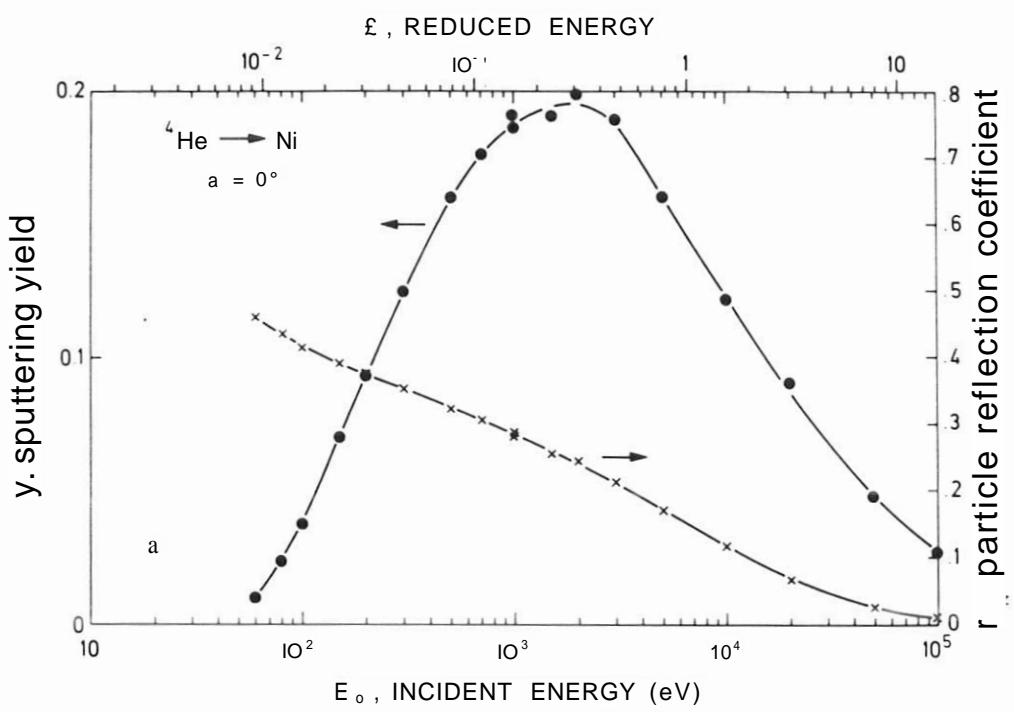


Fig. 9

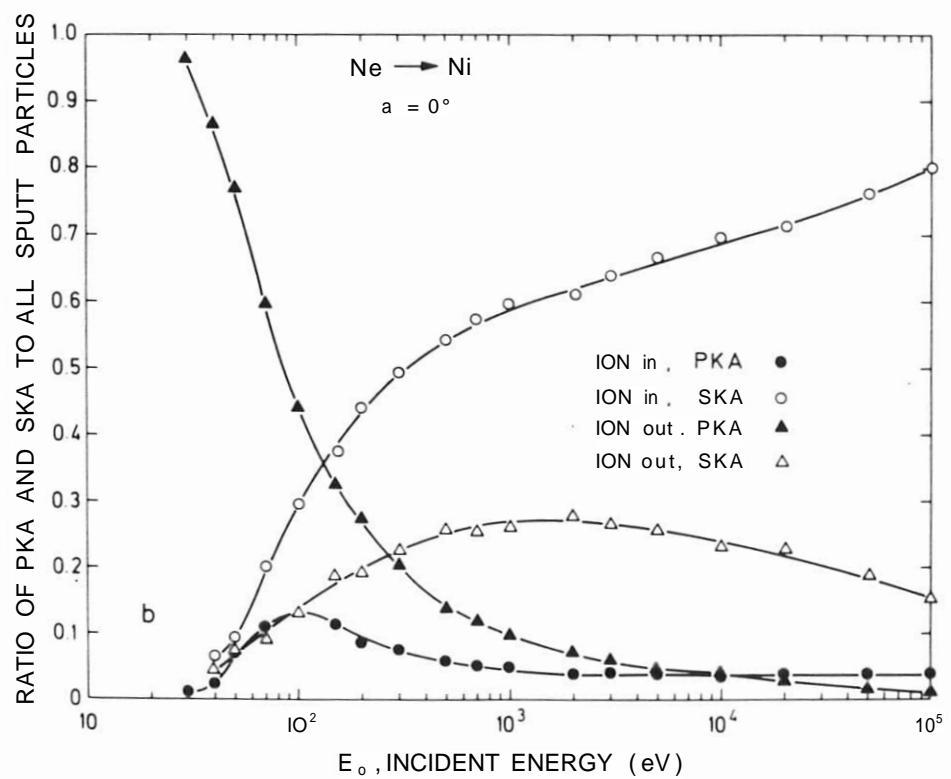
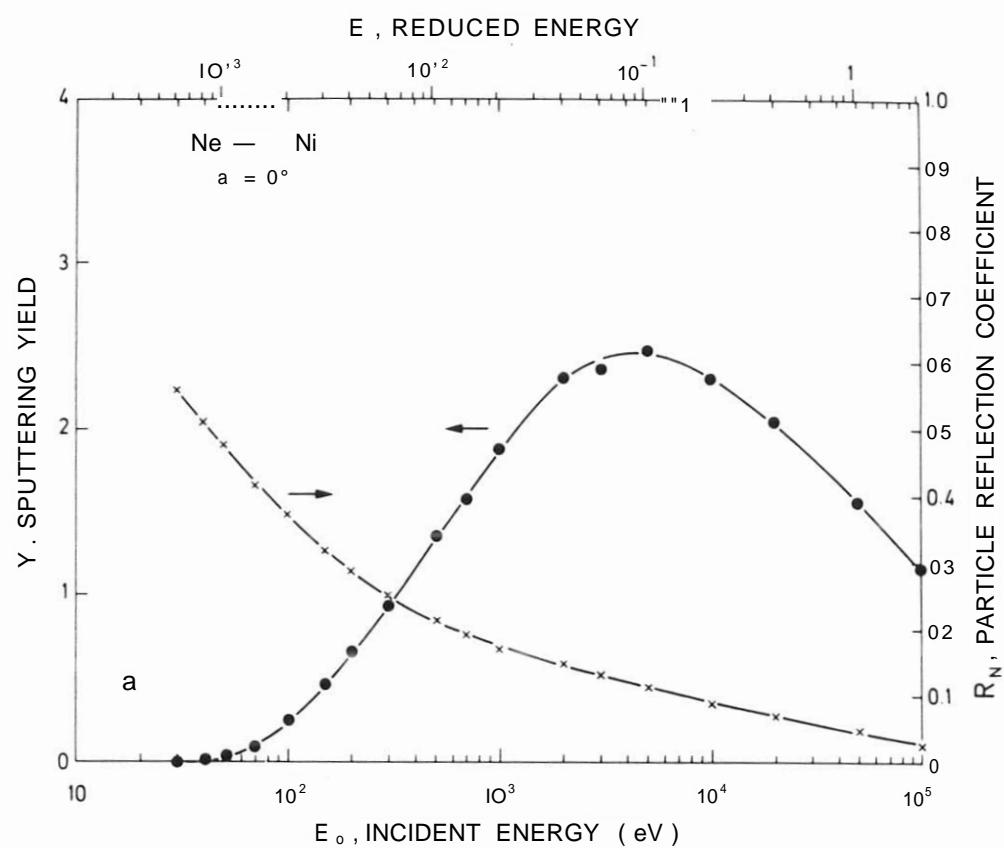


Fig. 10

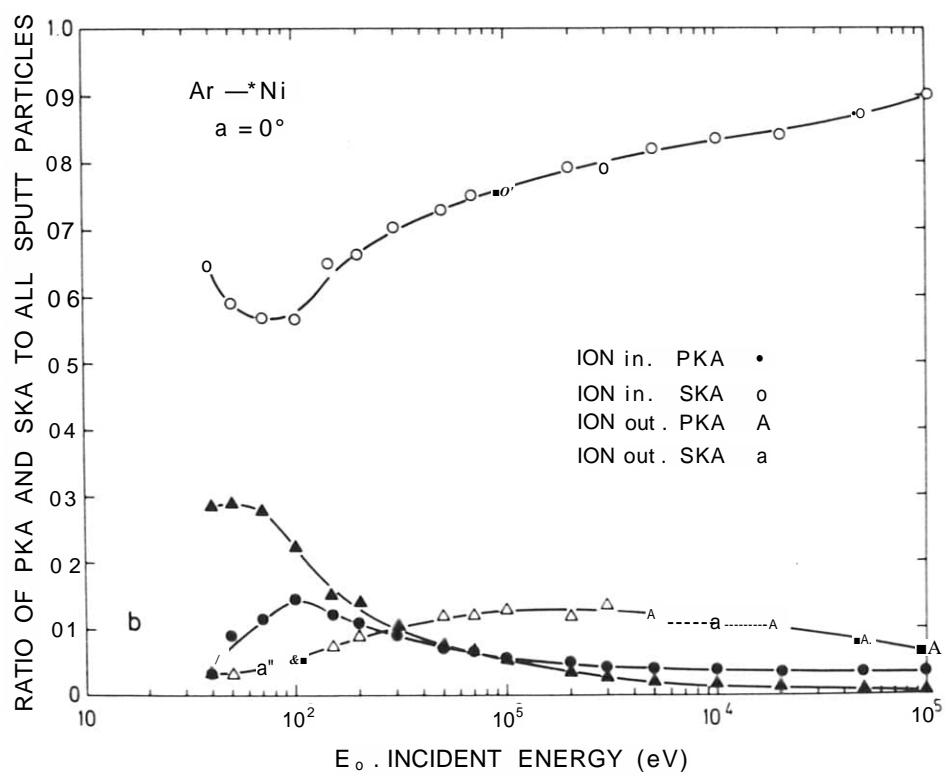
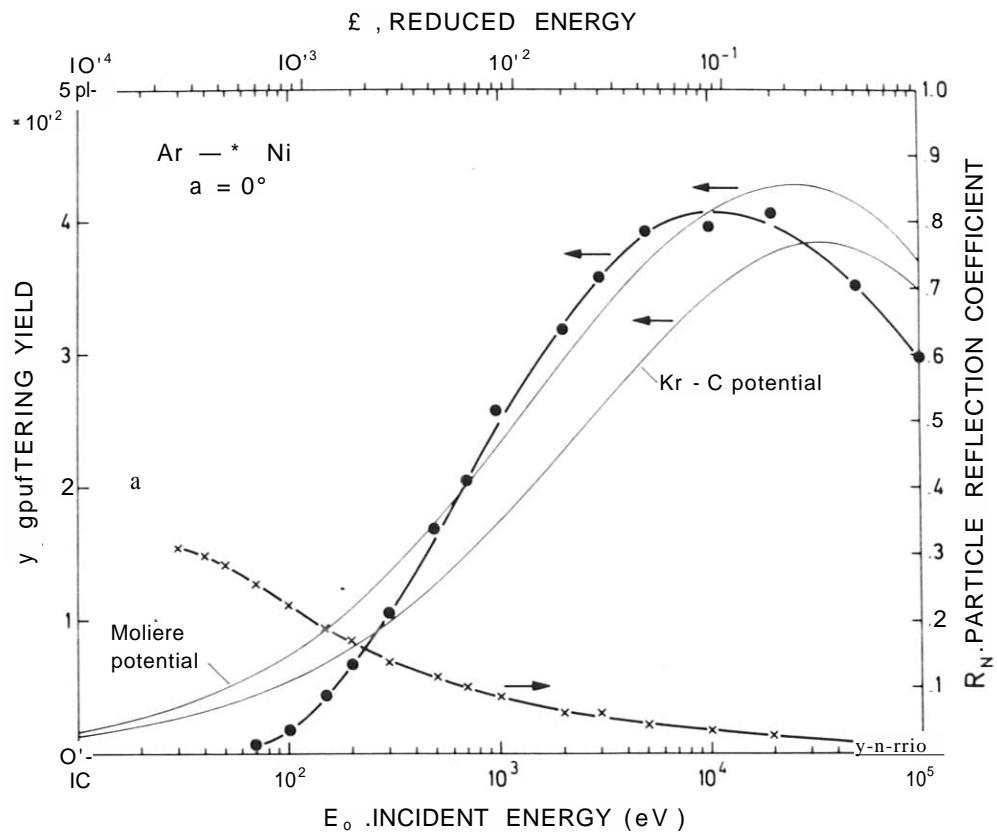


Fig . 11

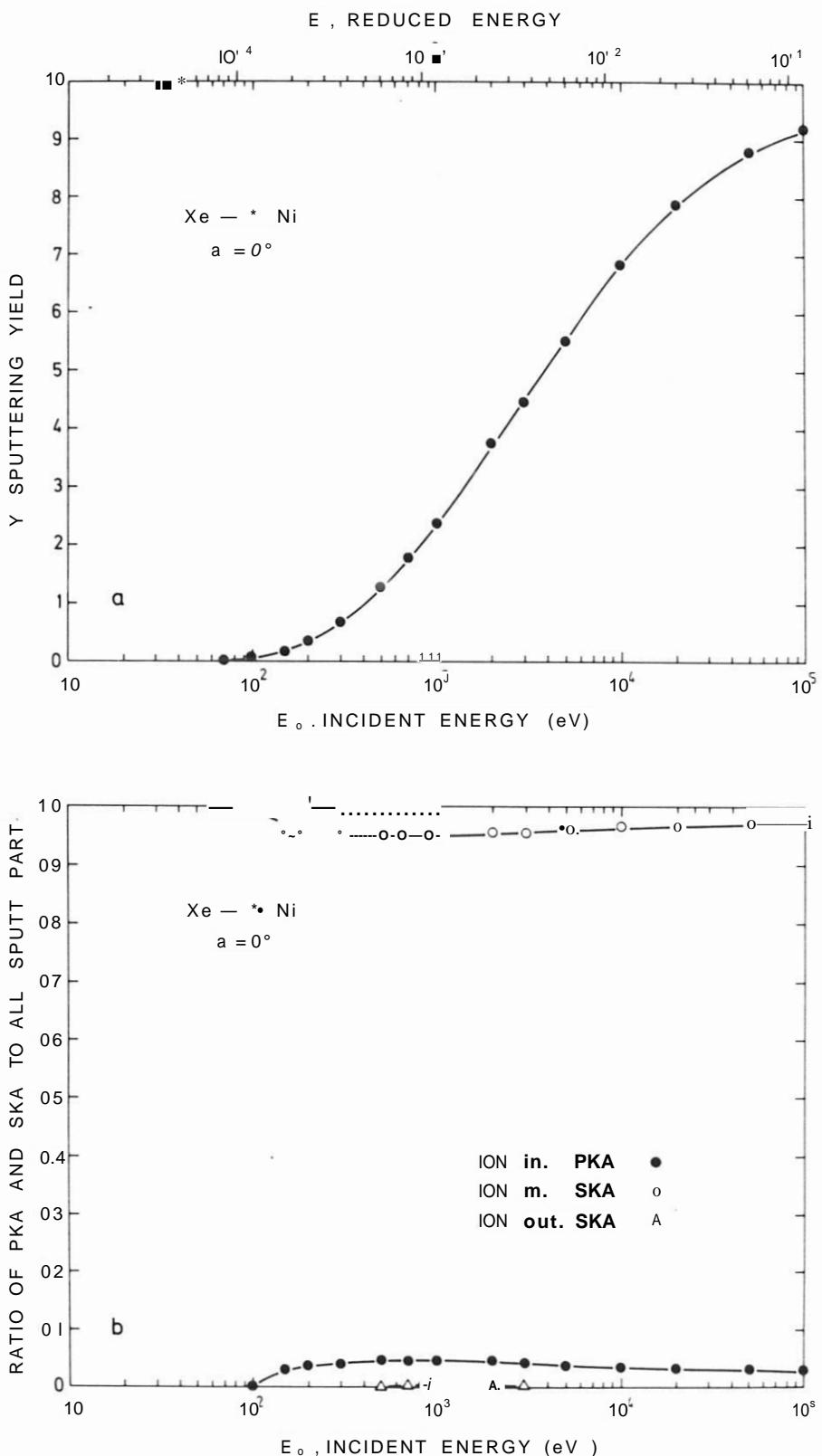


Fig . 12

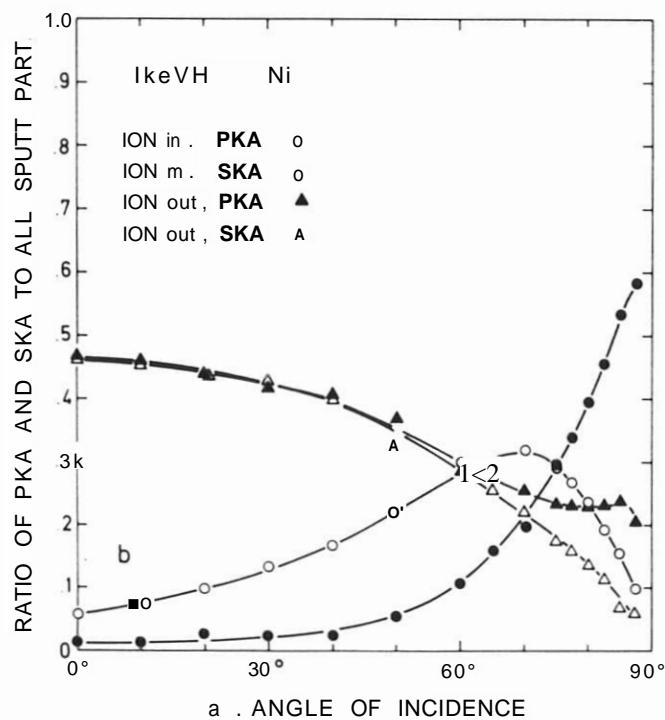
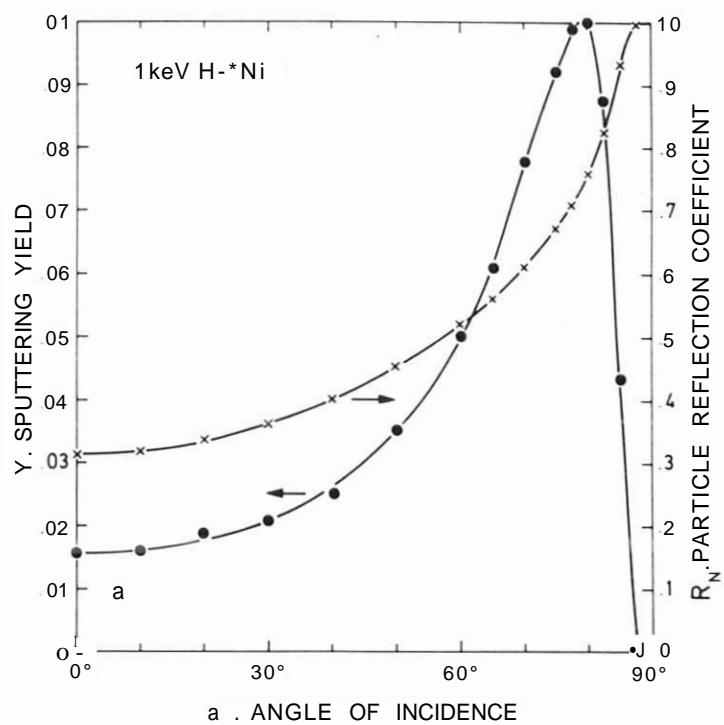


Fig. 13

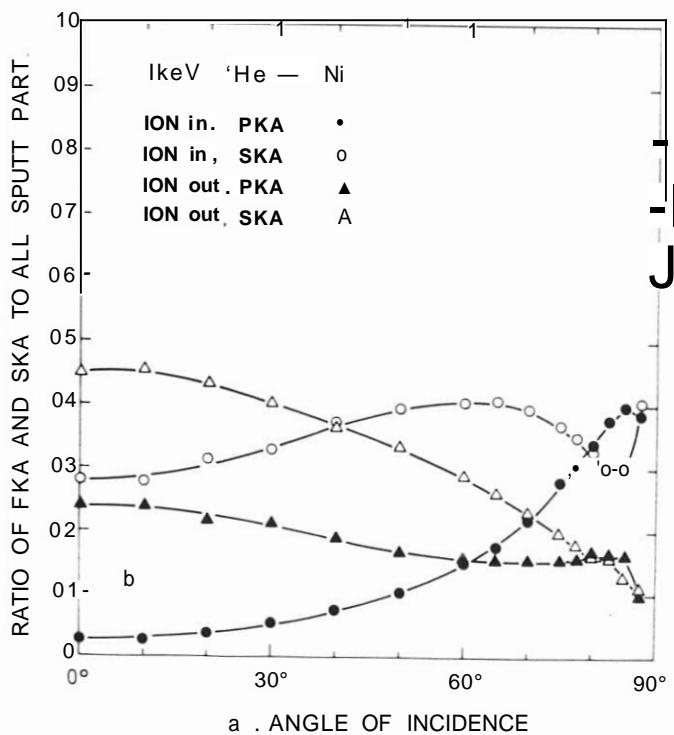
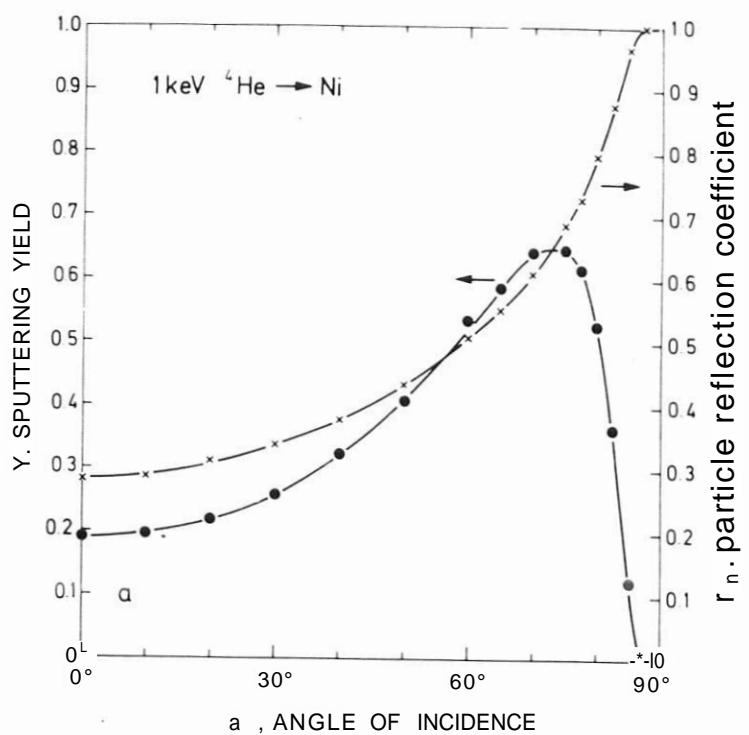


Fig. 14

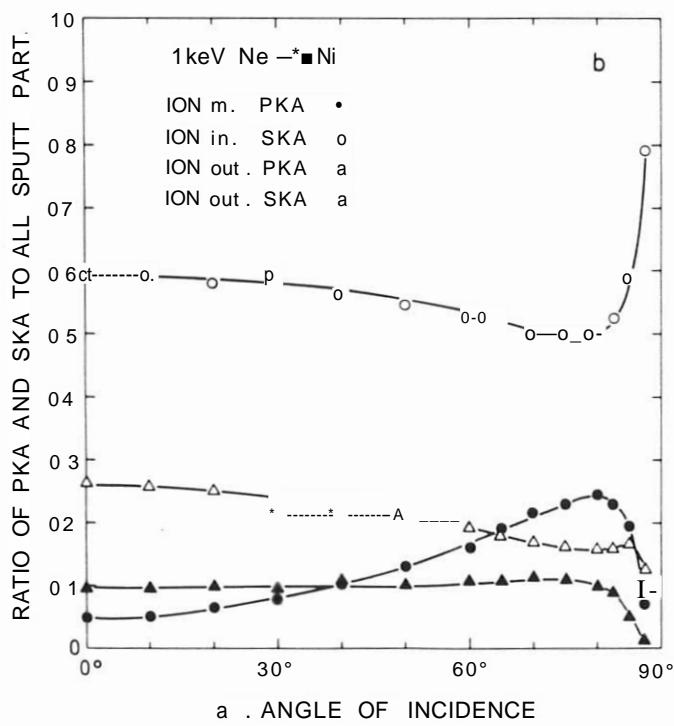
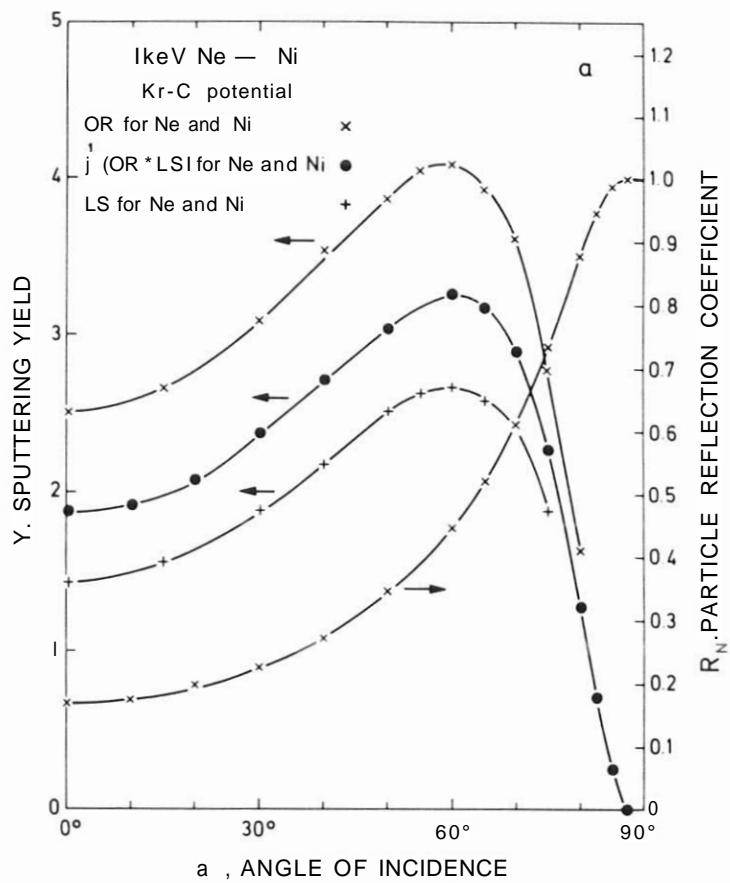


Fig. 15

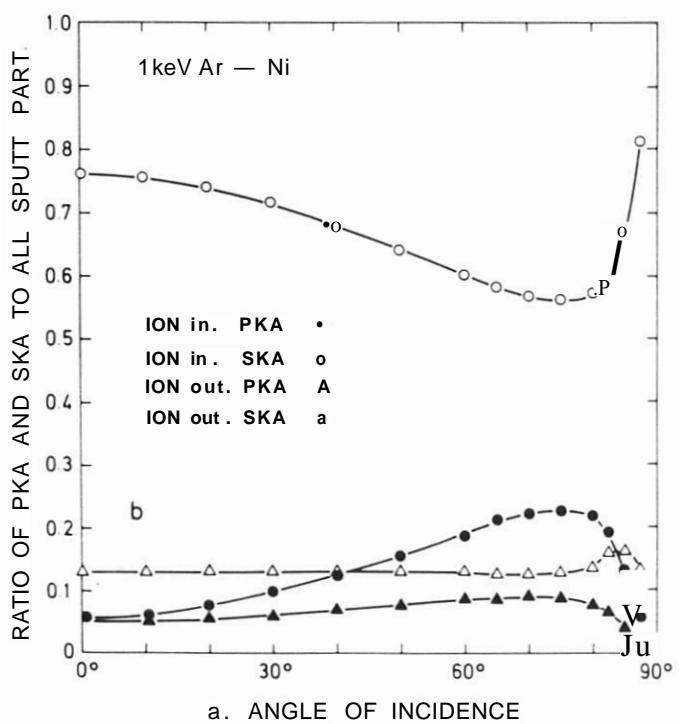
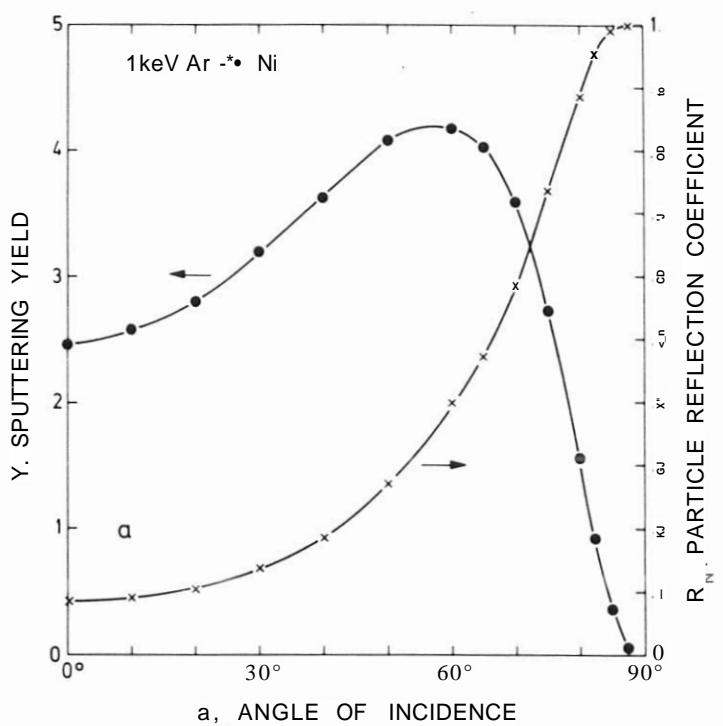


Fig. 16

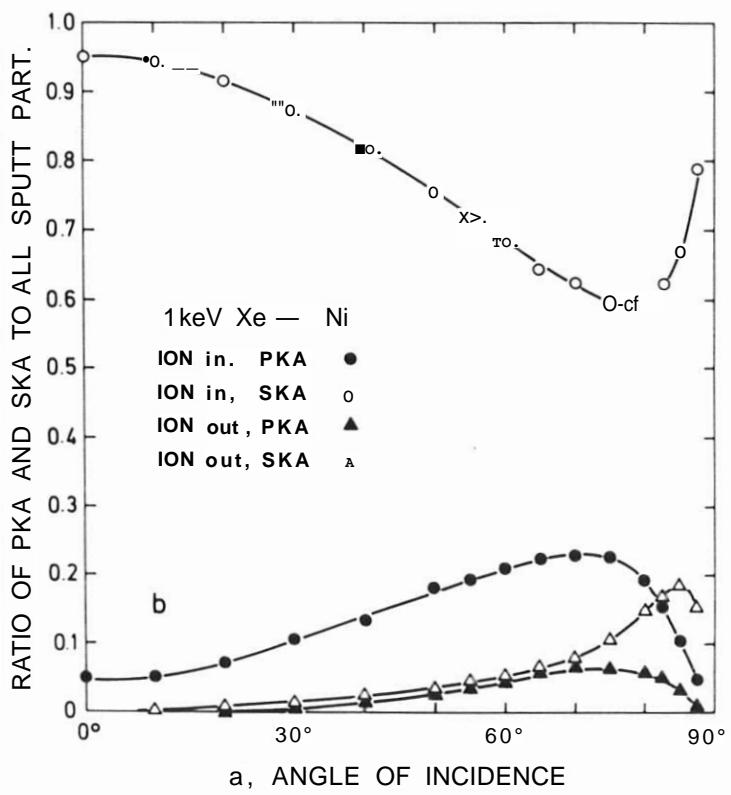
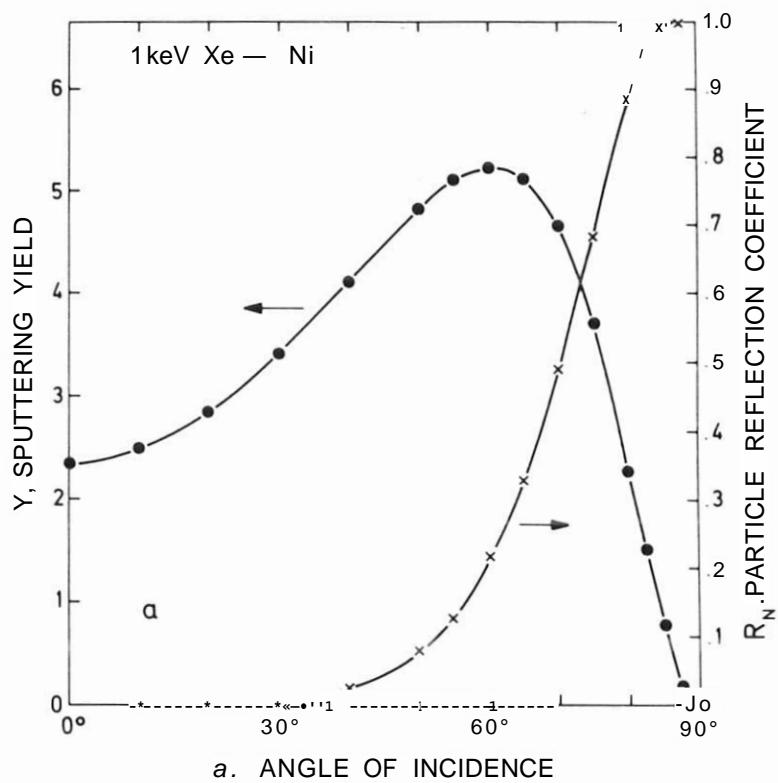


Fig. 17

a 13IA 9Ni331indS 'A

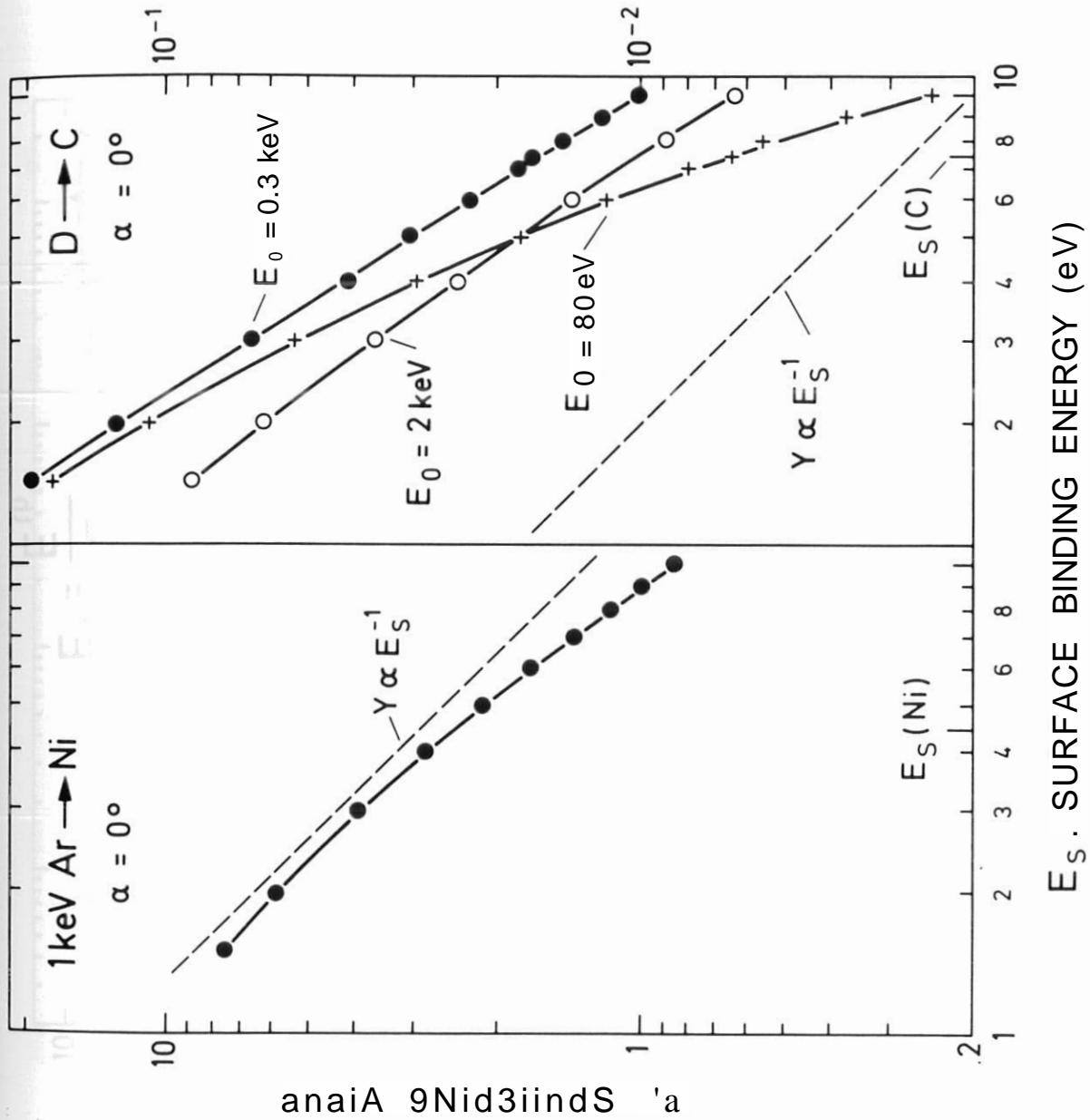


Fig. 18

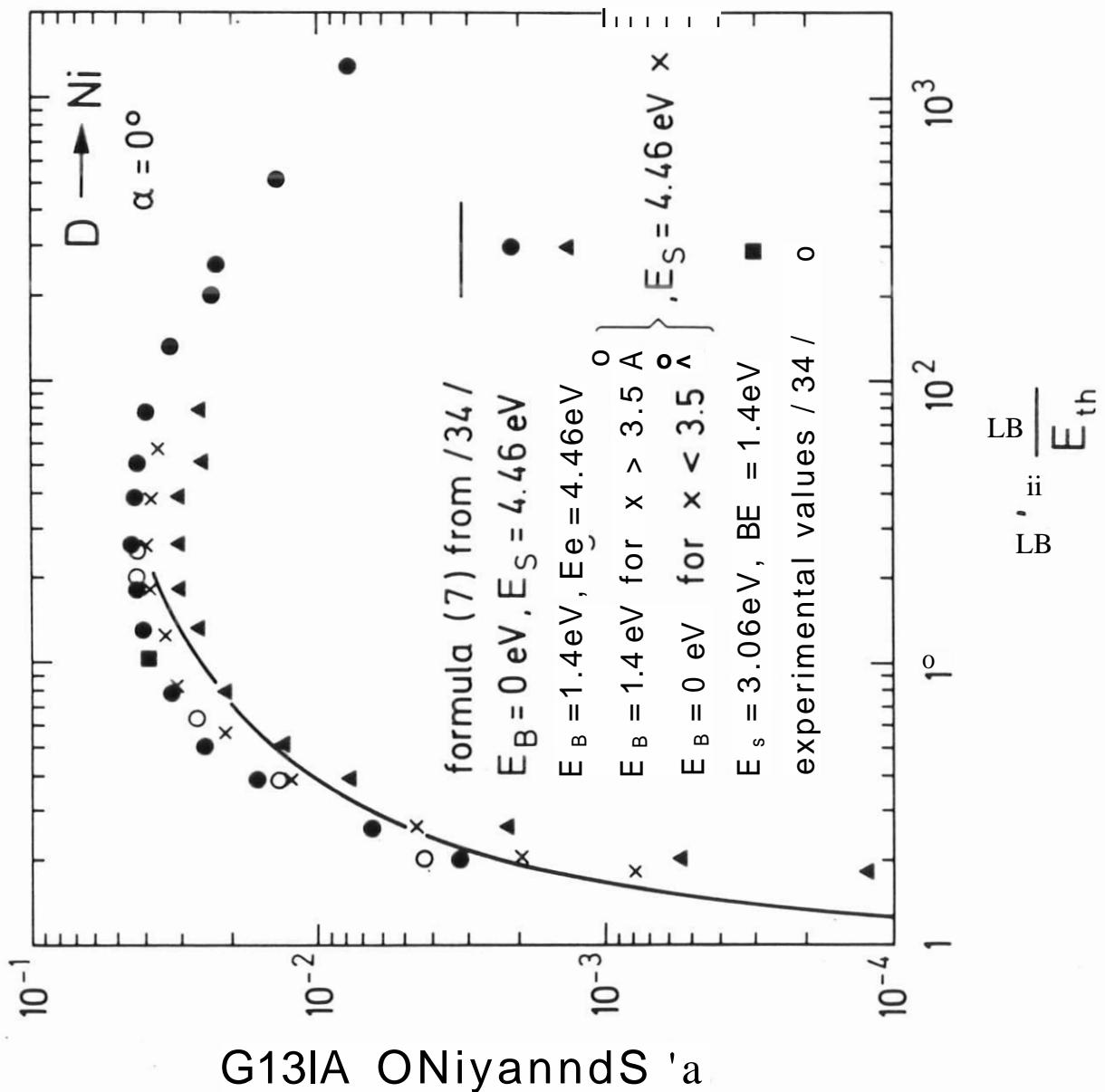


Fig. 19

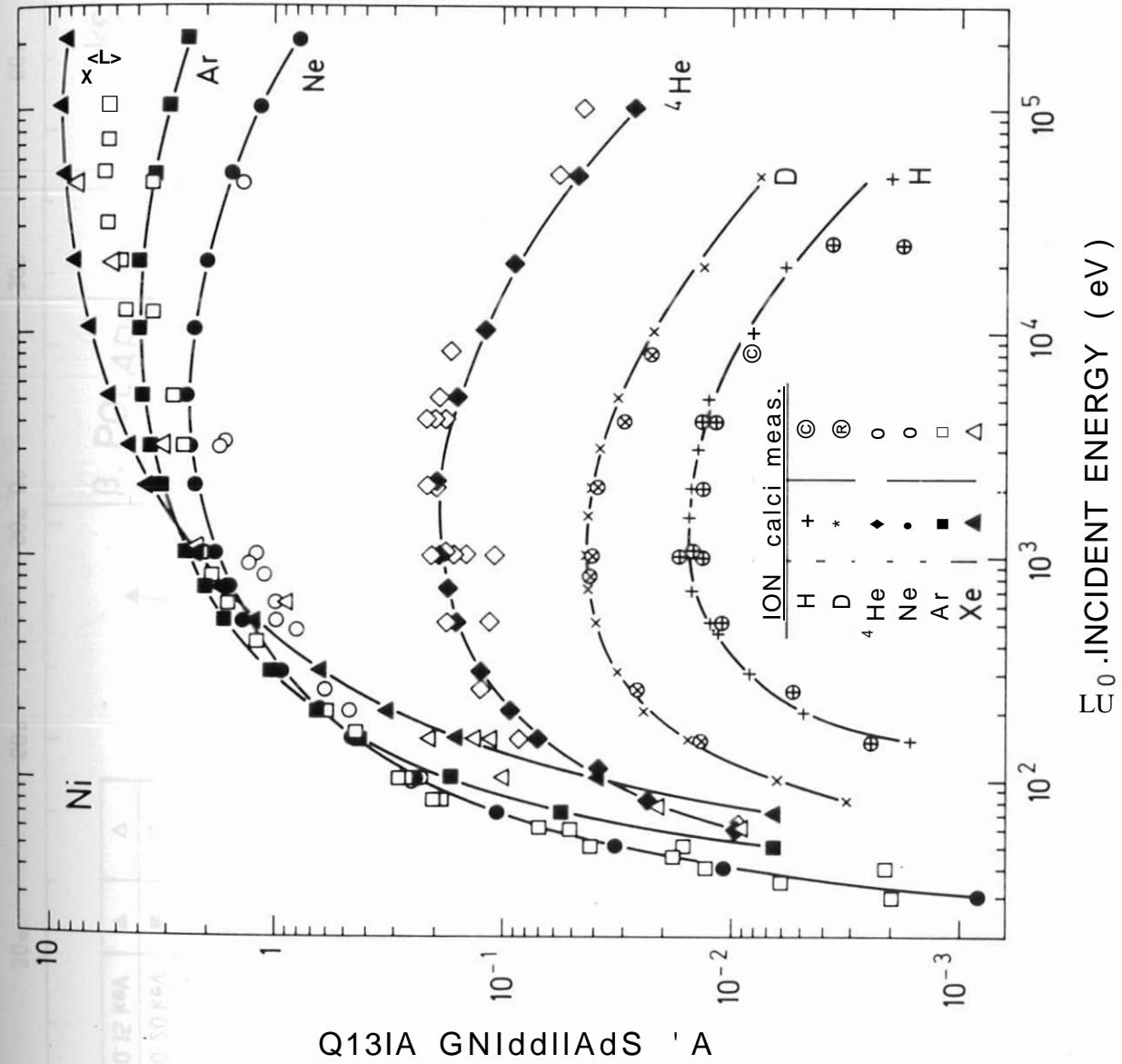


Fig. 20

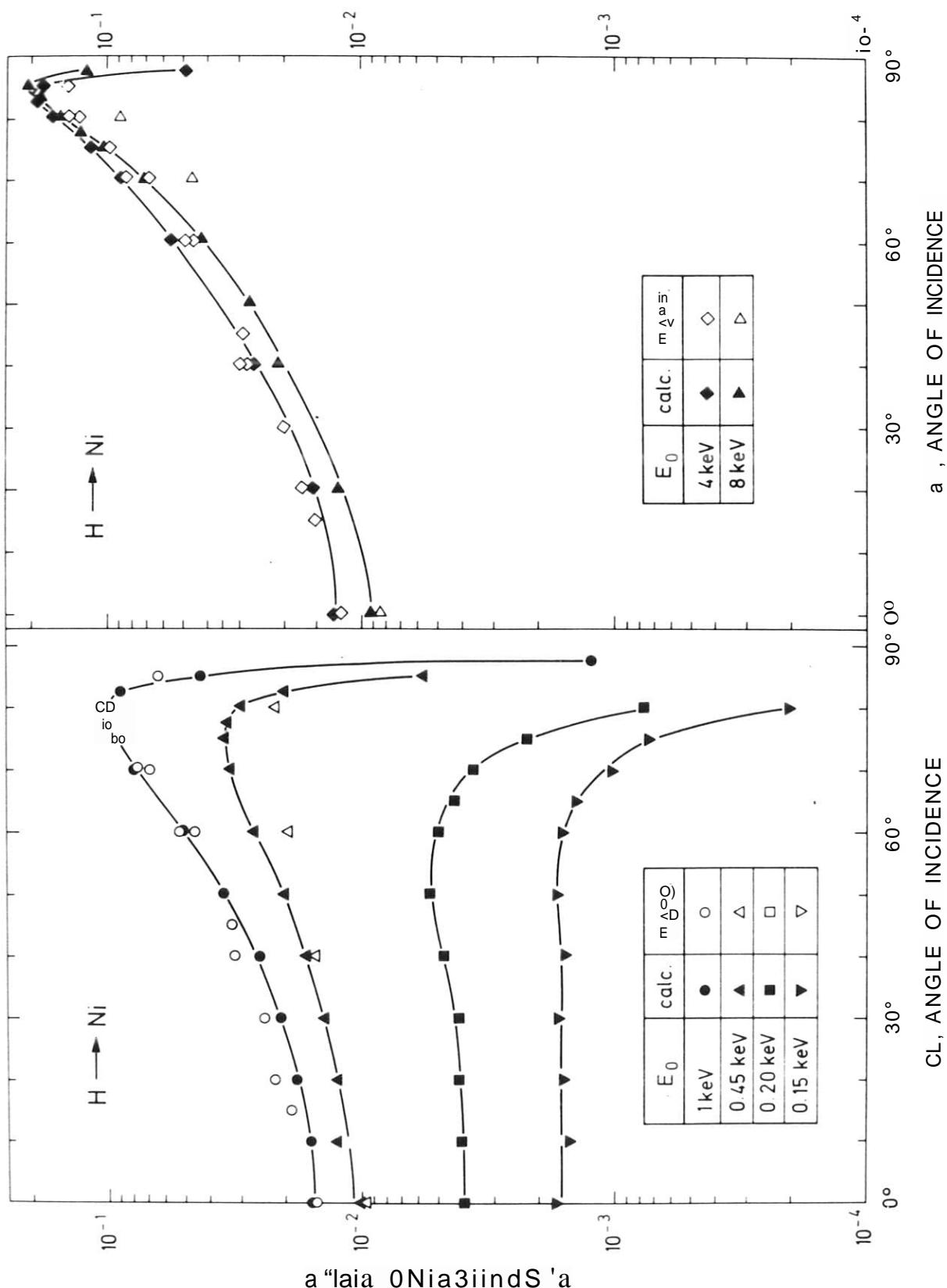


Fig. 21

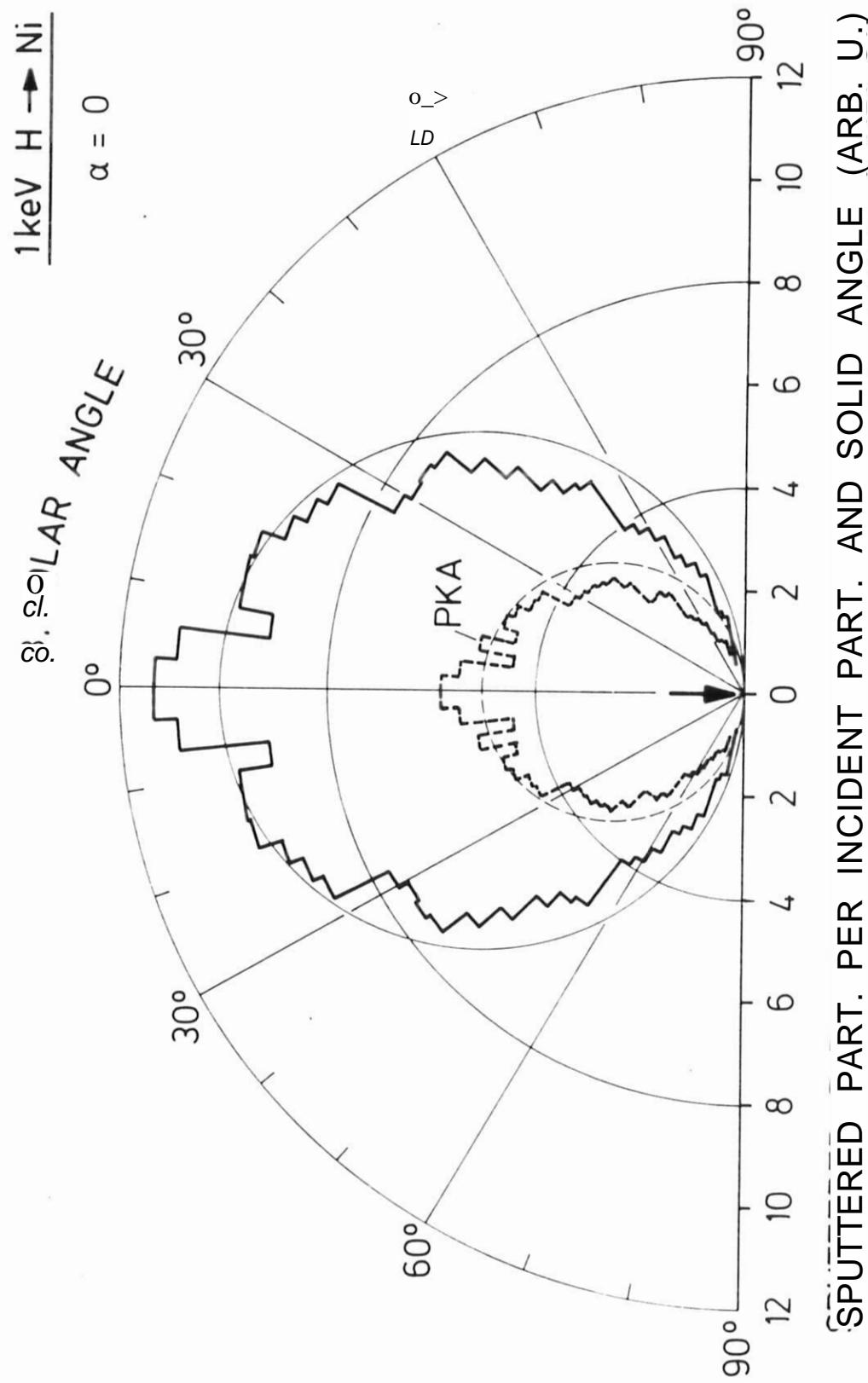


Fig. 22

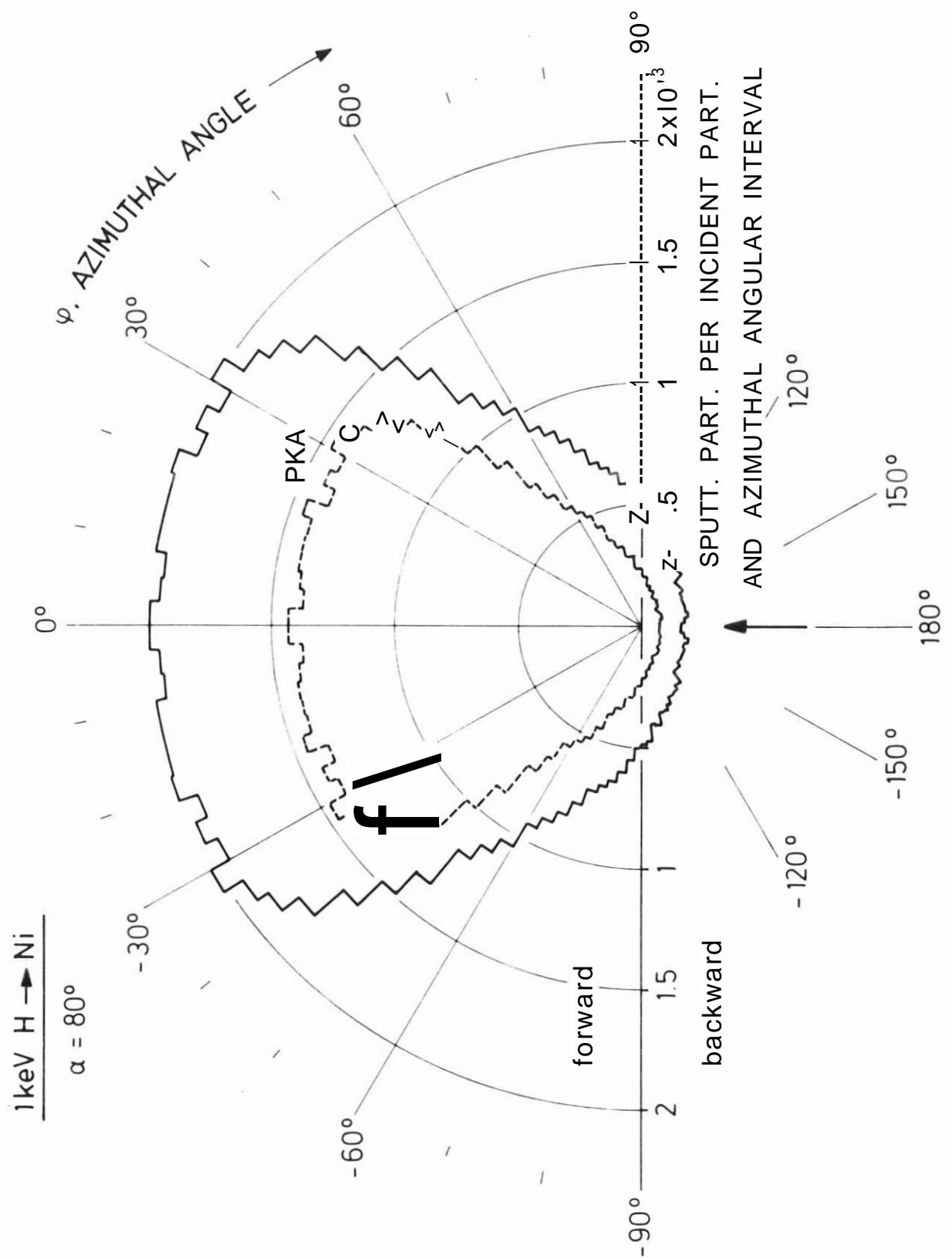


Fig. 23

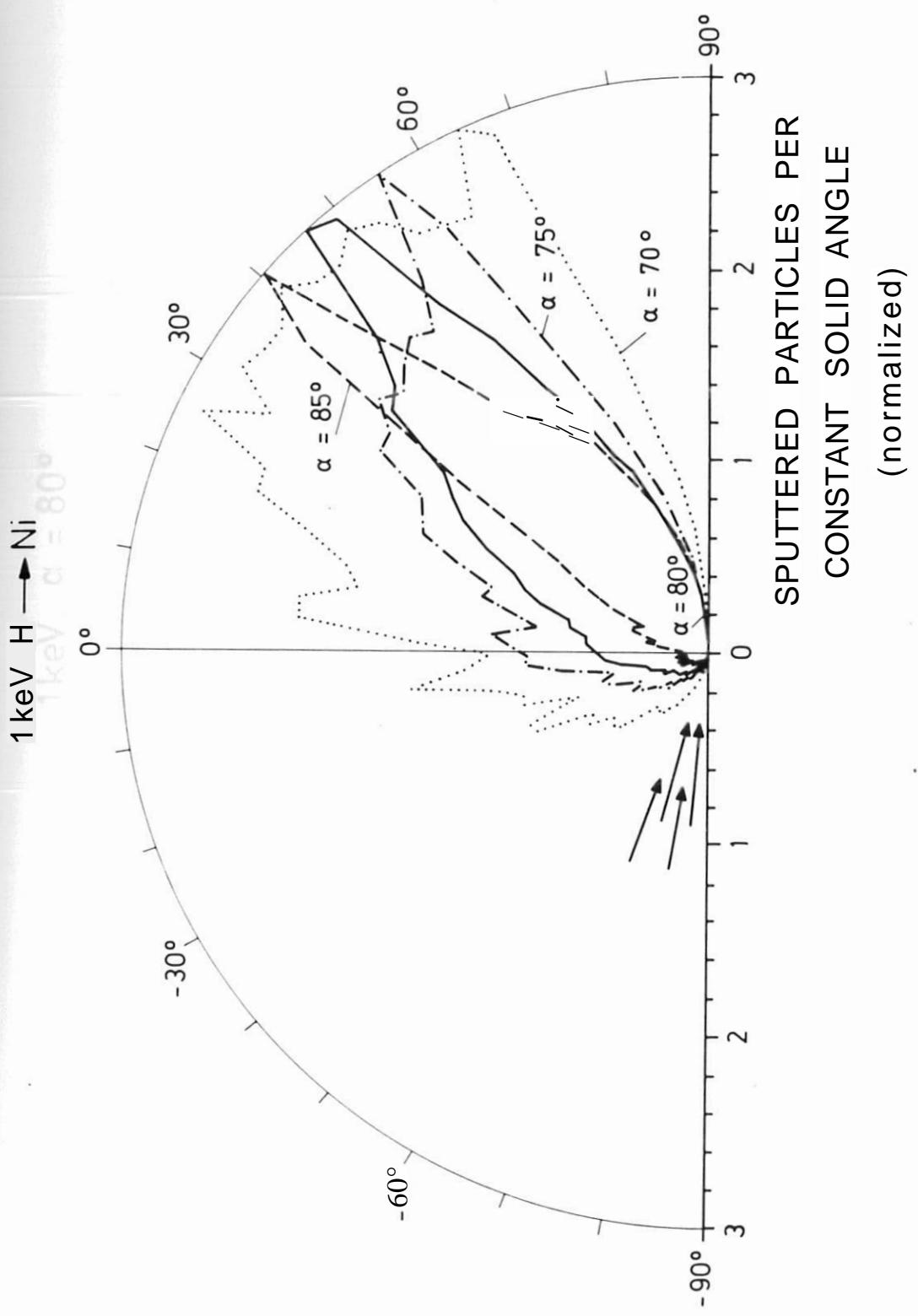


Fig. 24

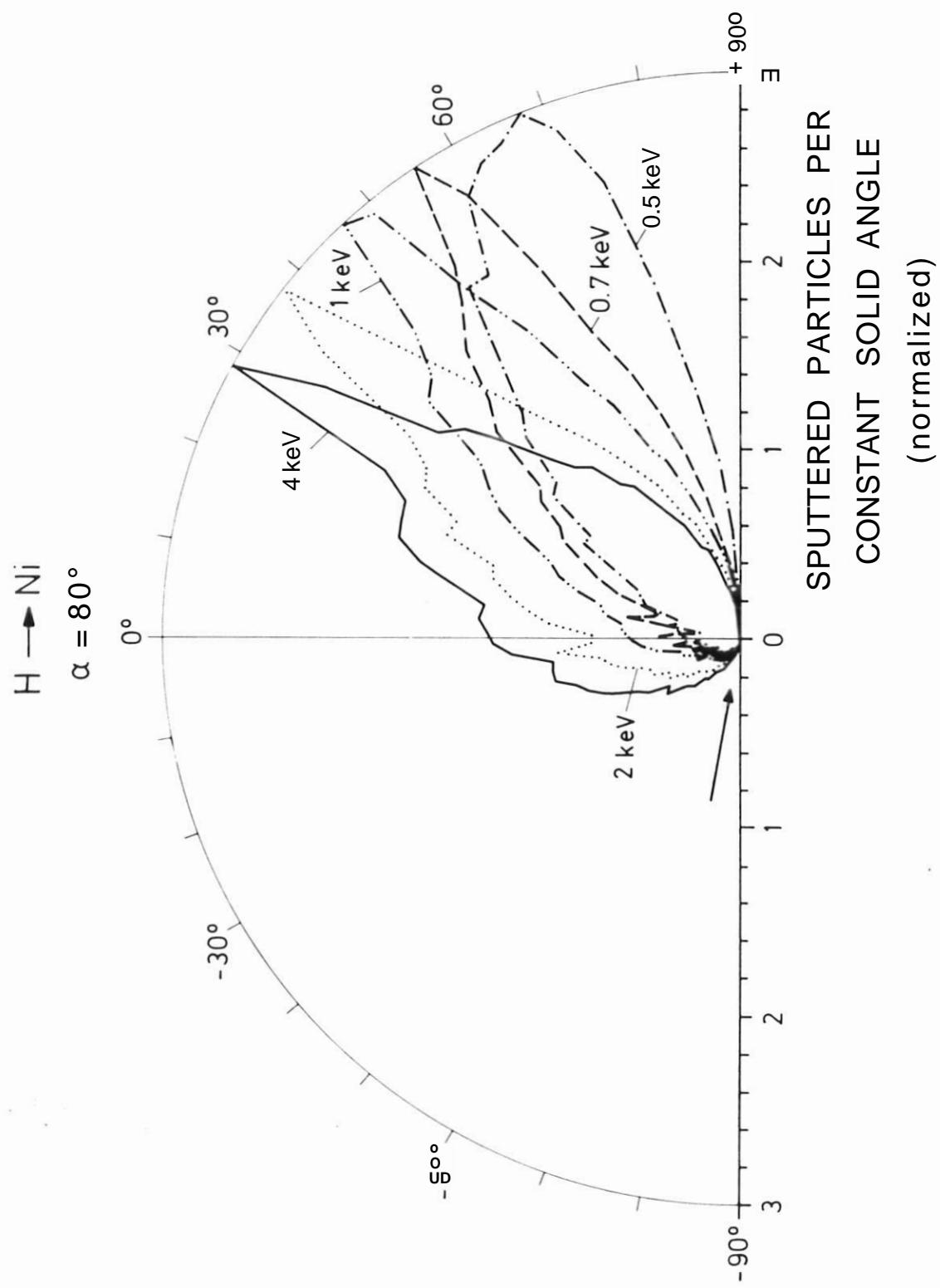


Fig. 25

$1\text{keV}, \alpha = 80^\circ$

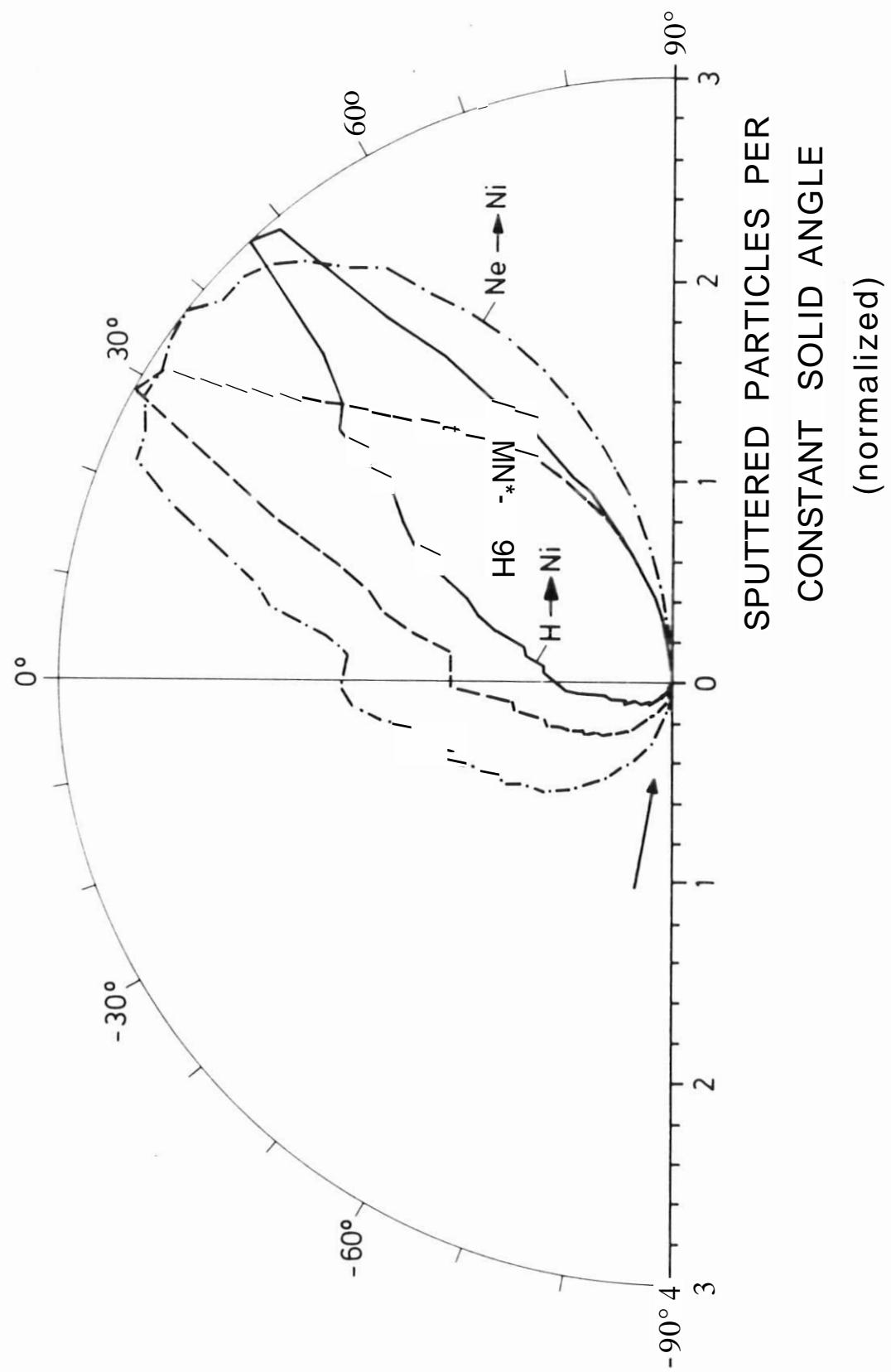


Fig. 26

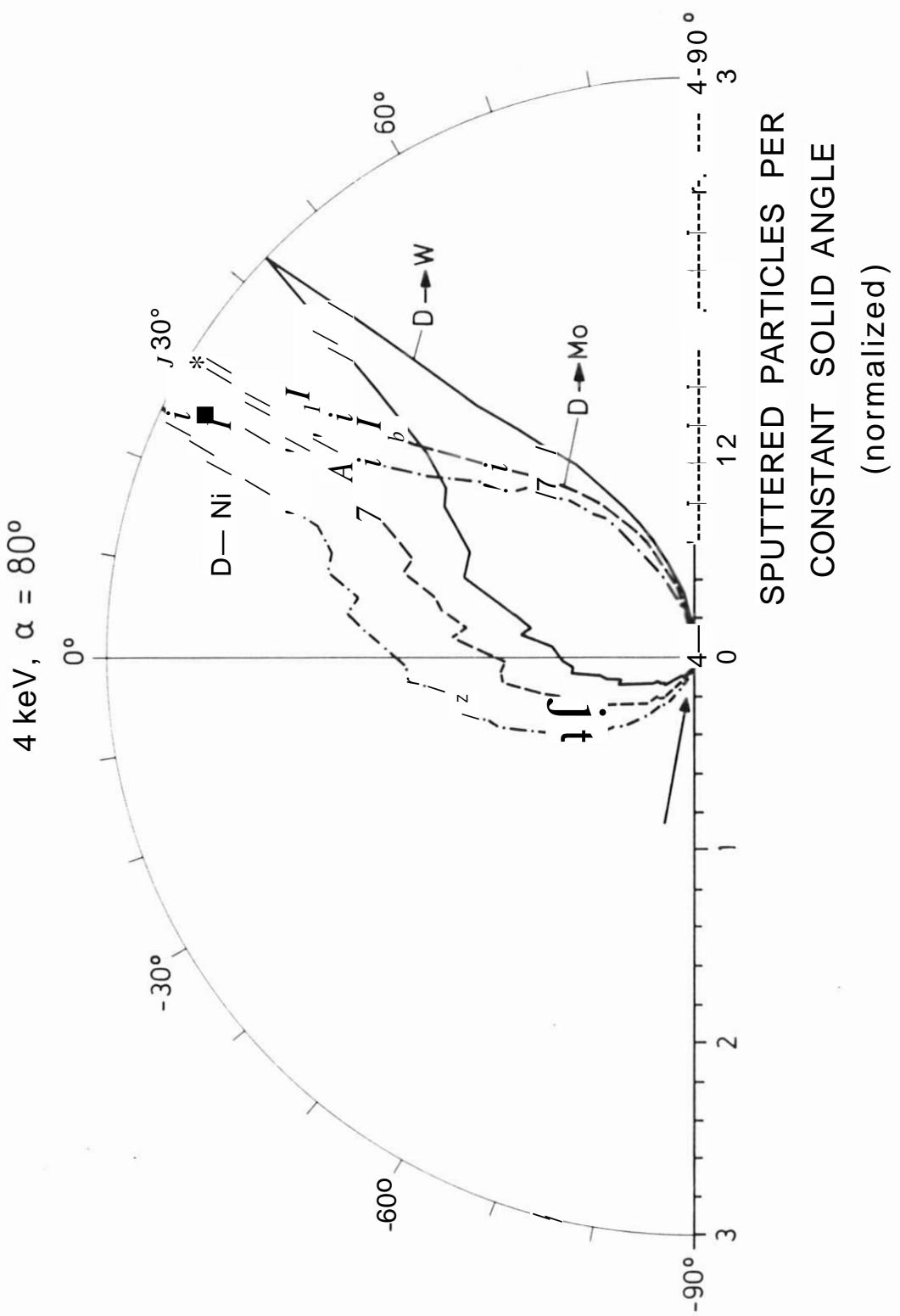


Fig. 27

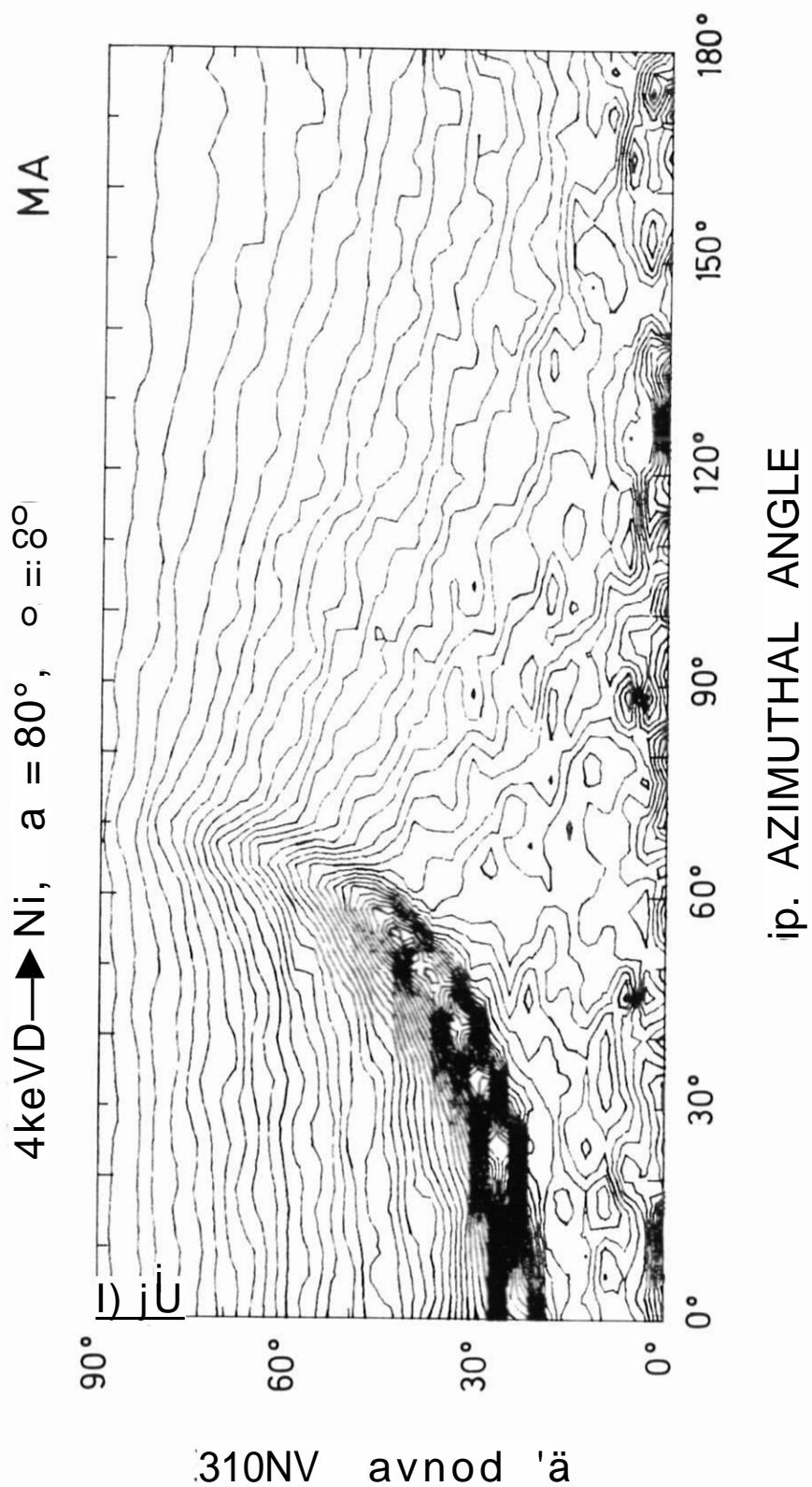


Fig. 28a

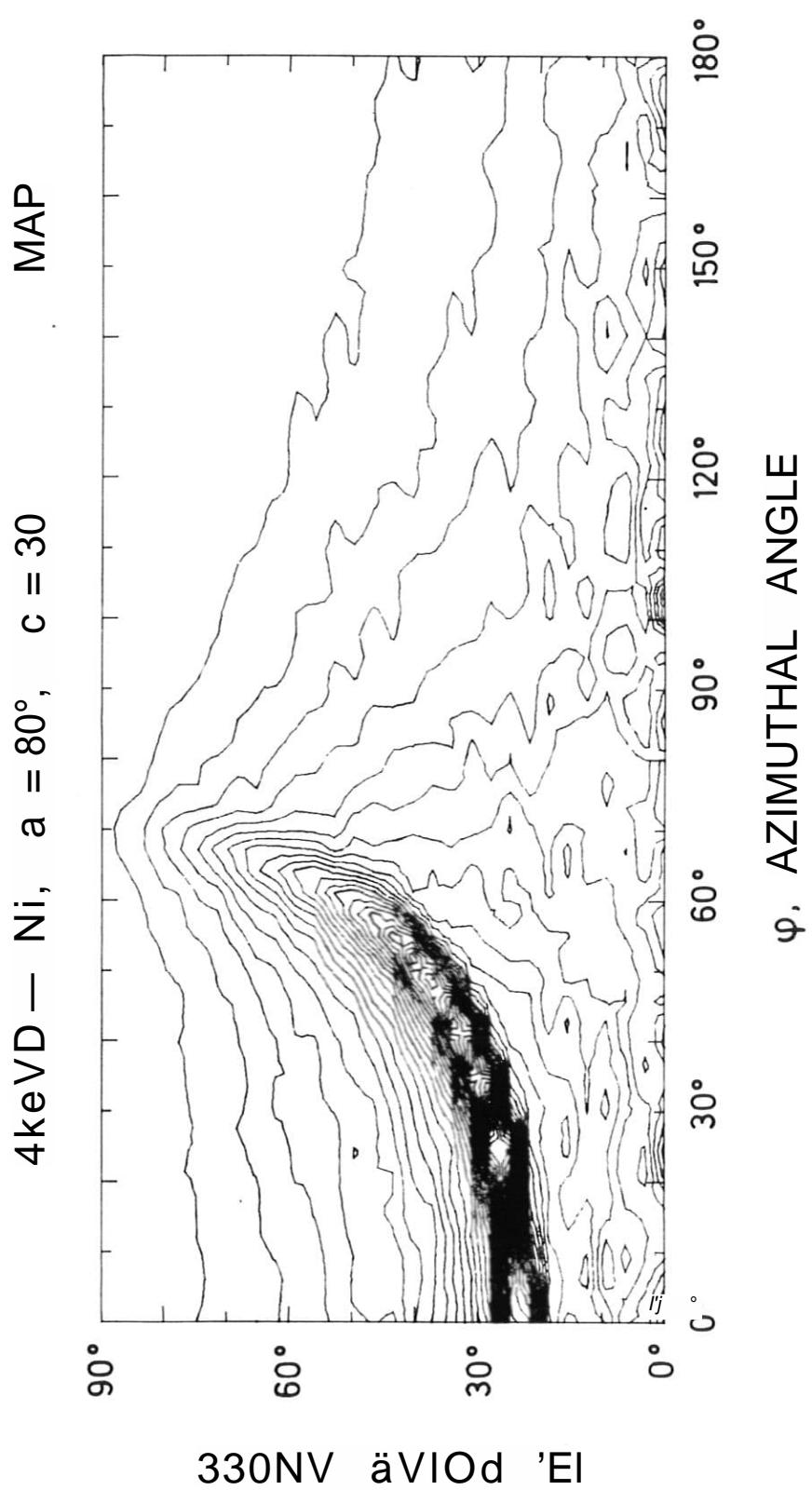


Fig. 28b

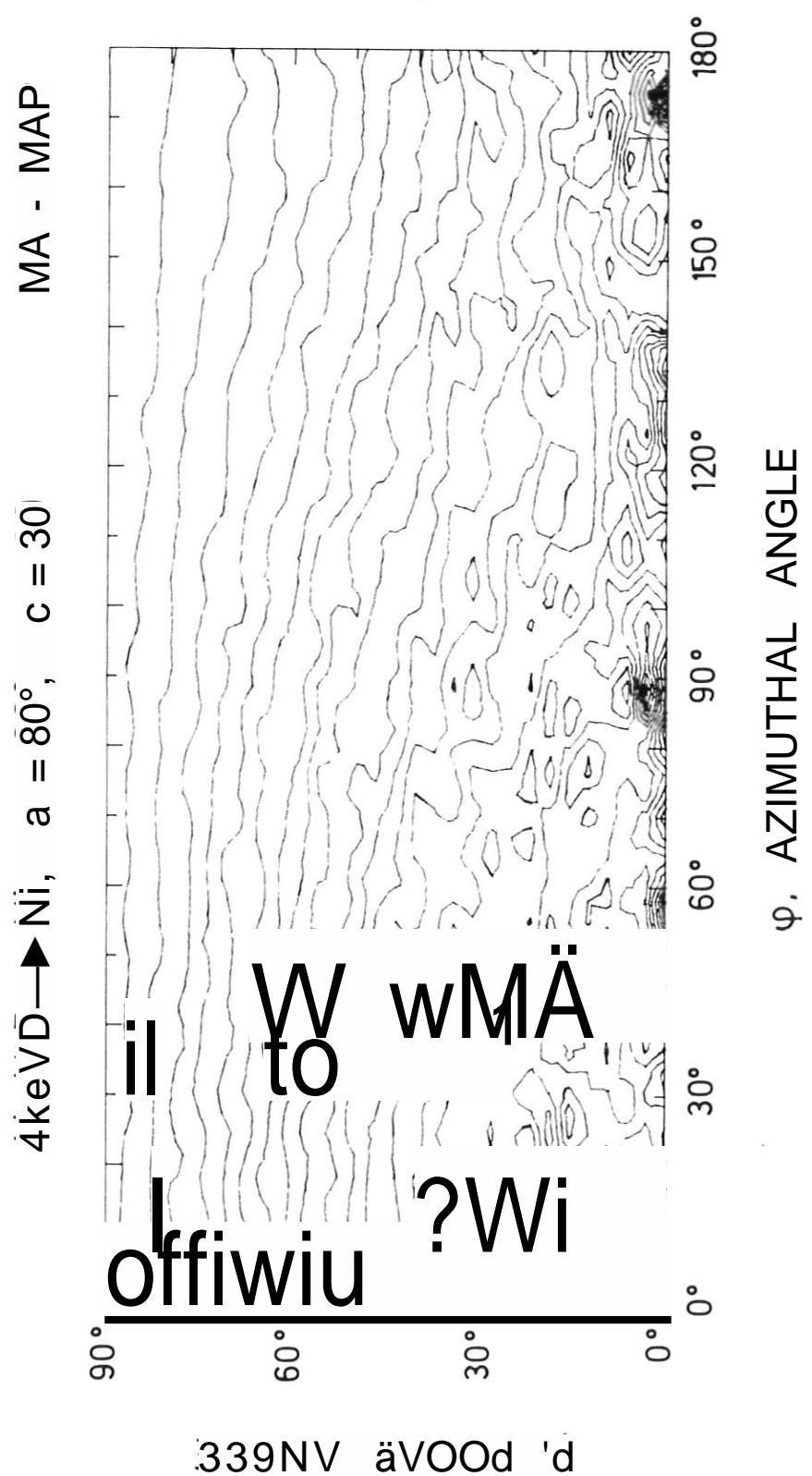


Fig. 28c

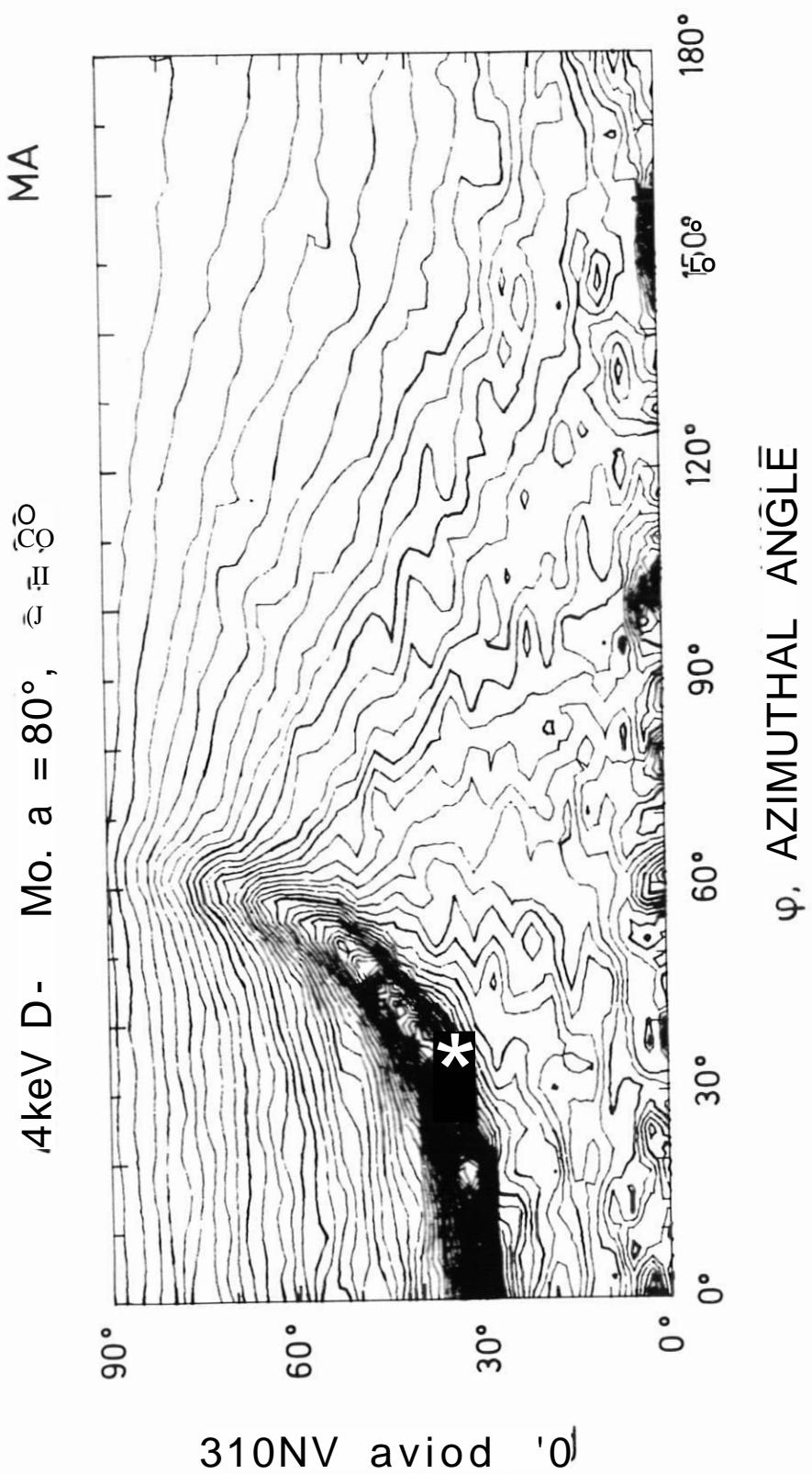
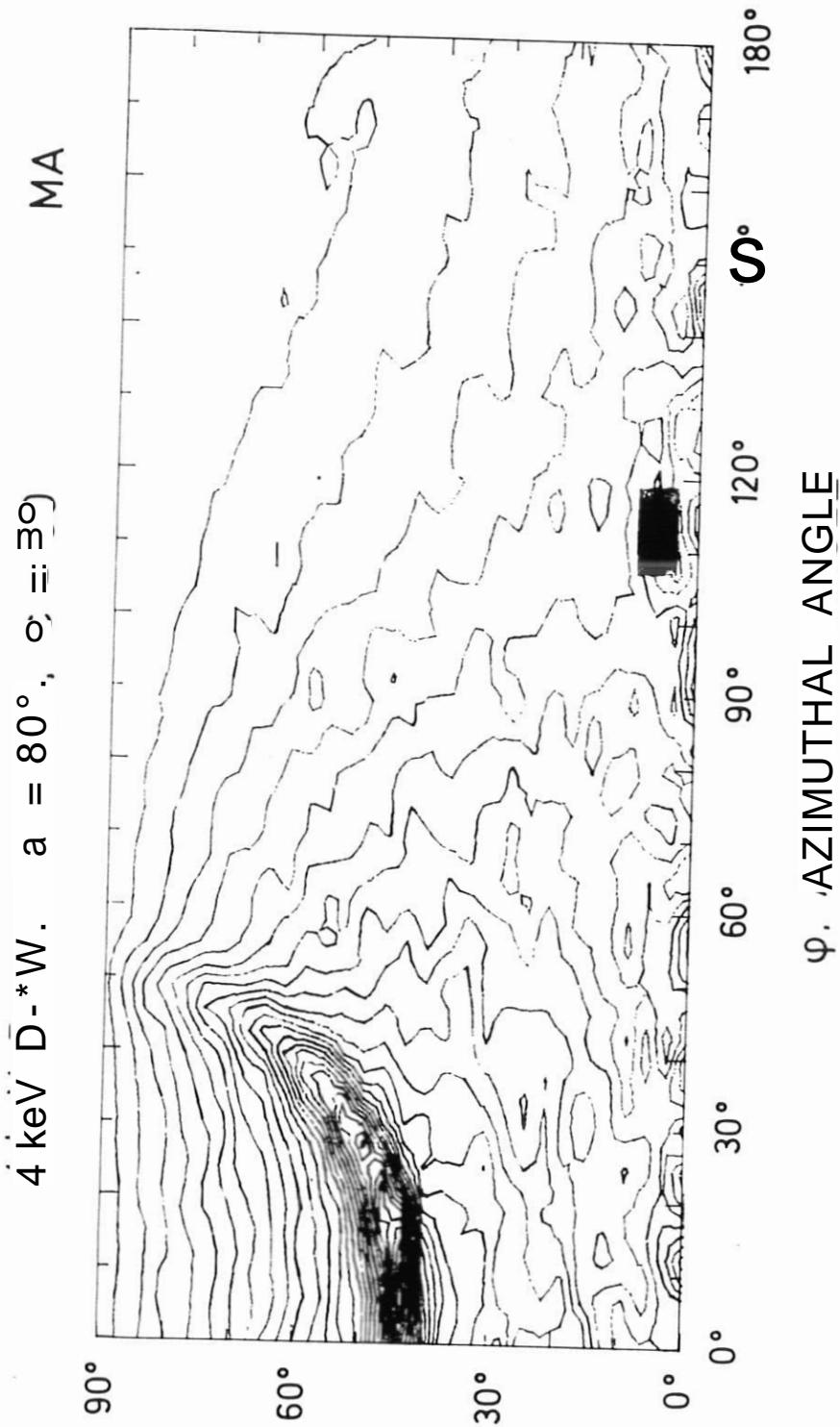


Fig. 299



310NV aviod 'd

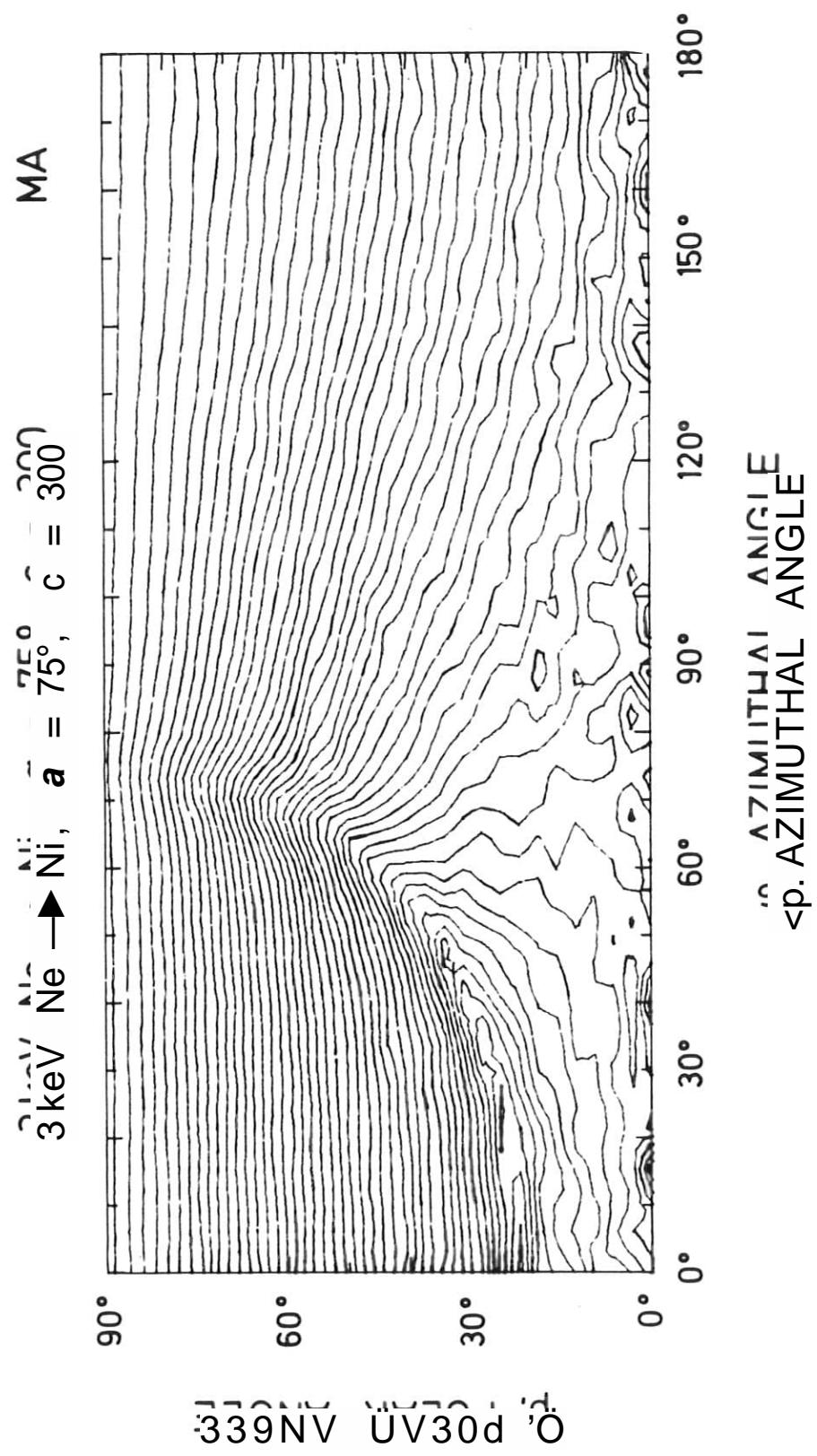
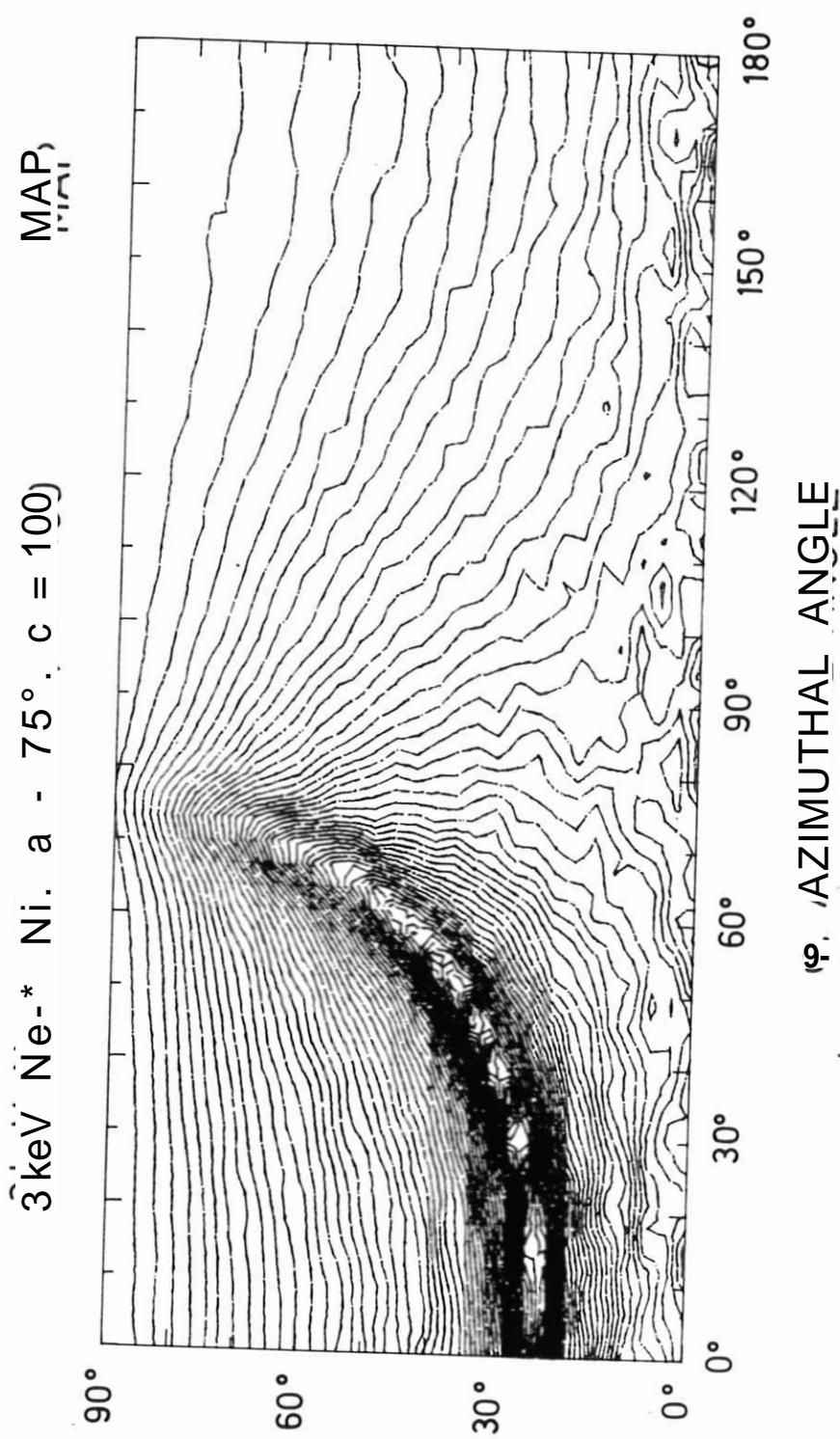


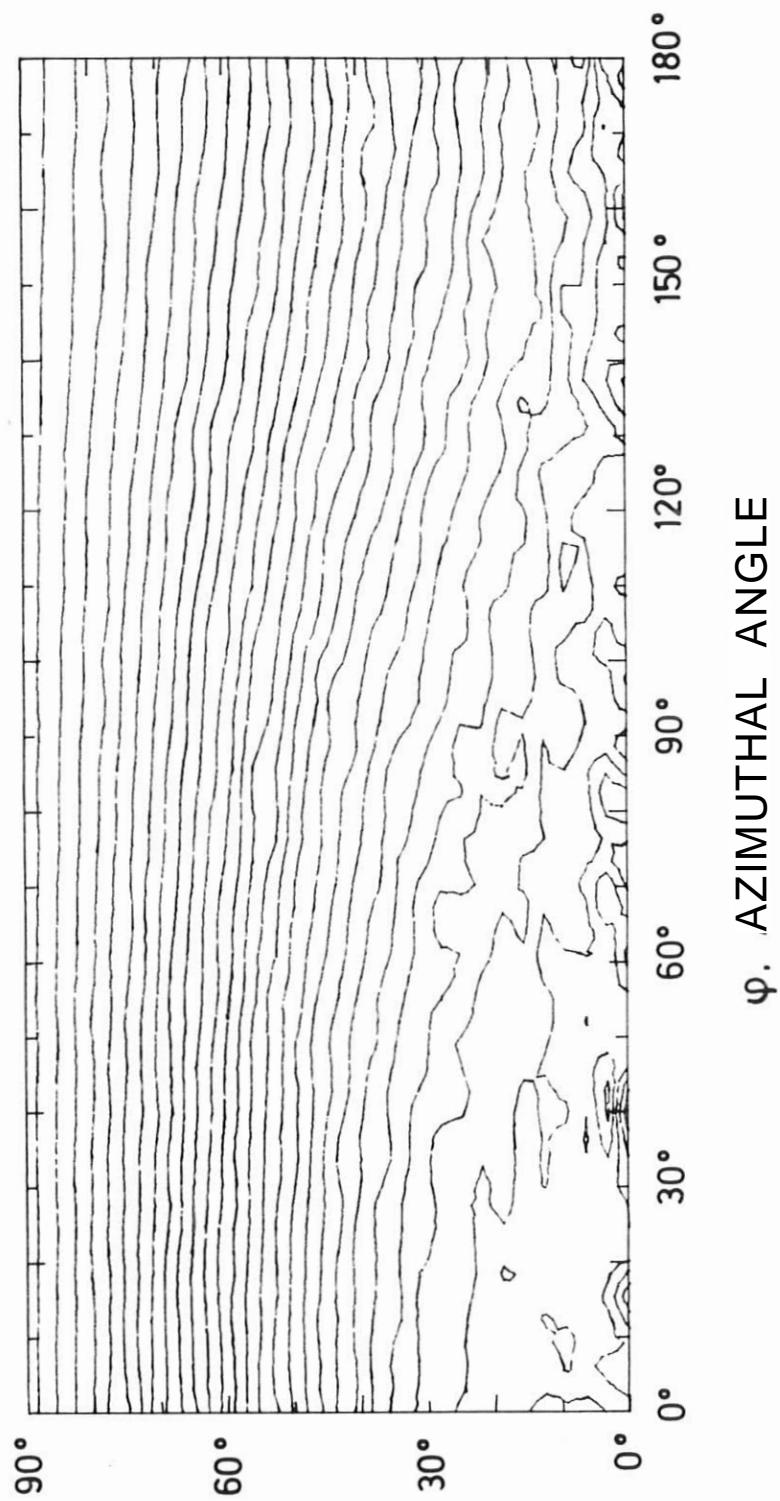
Fig. 31a



-319NV dVIOD 'd

Fig. 31b

3 keV Ne  $\rightarrow$  Ni.  $a = 75^\circ$ , c - 300 MA - MAP



.310NV avnod 'd

Fig. 31c

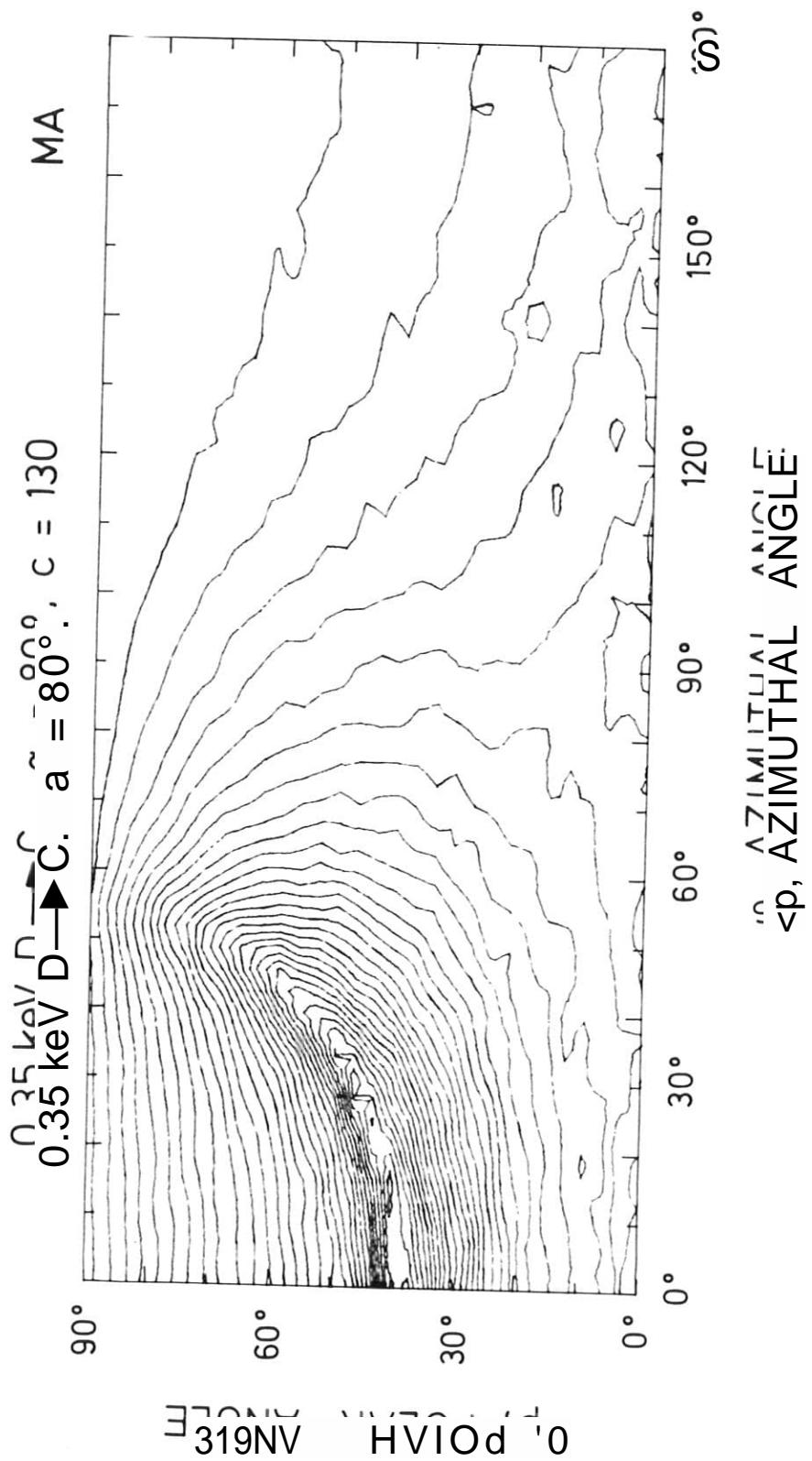


Fig. 32a

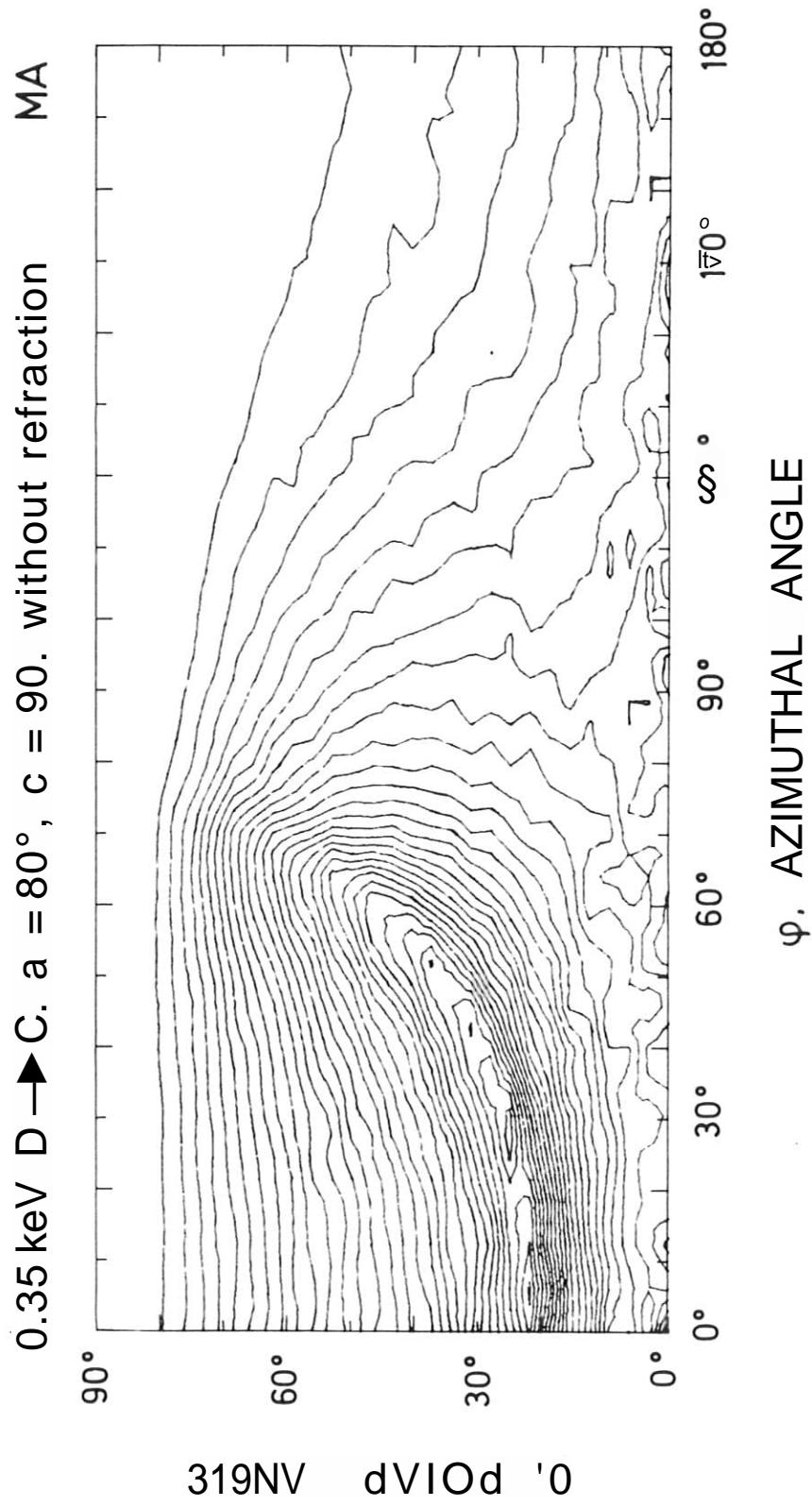


Fig. 32b

$0.35 \text{ keV D-} \rightarrow \text{C}$   
 $\alpha = 80^\circ$

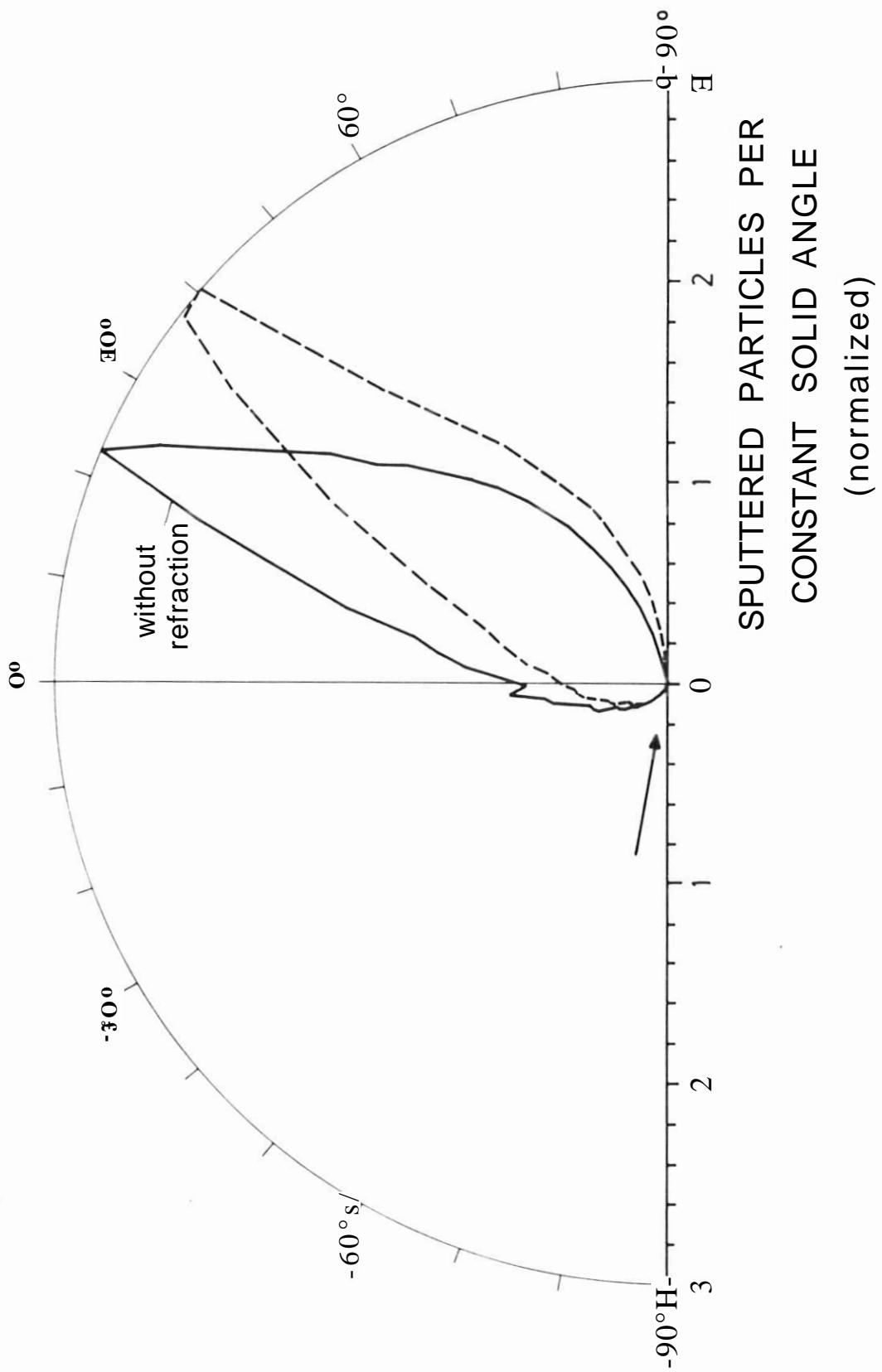


Fig. 33

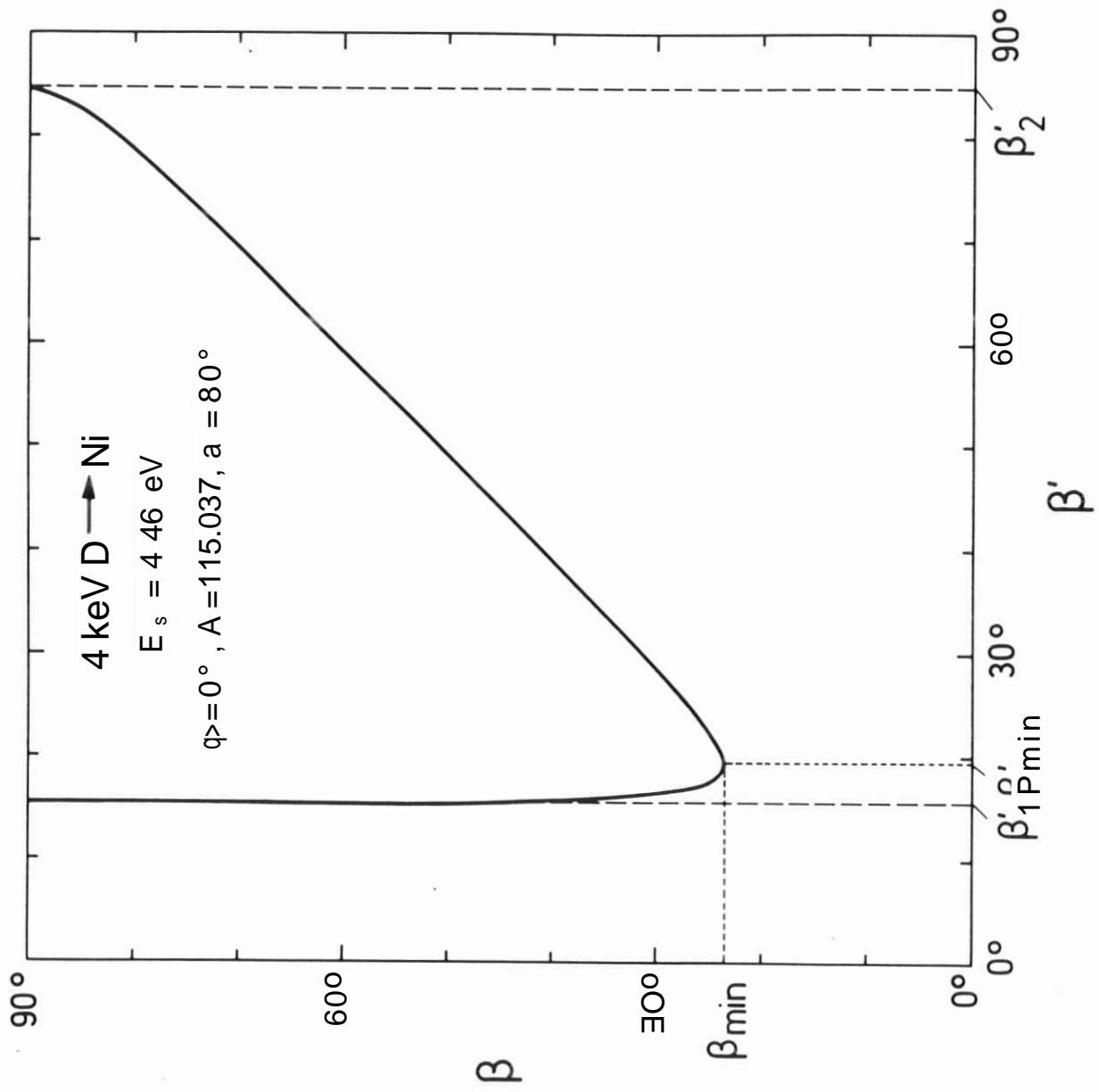


Fig. 34

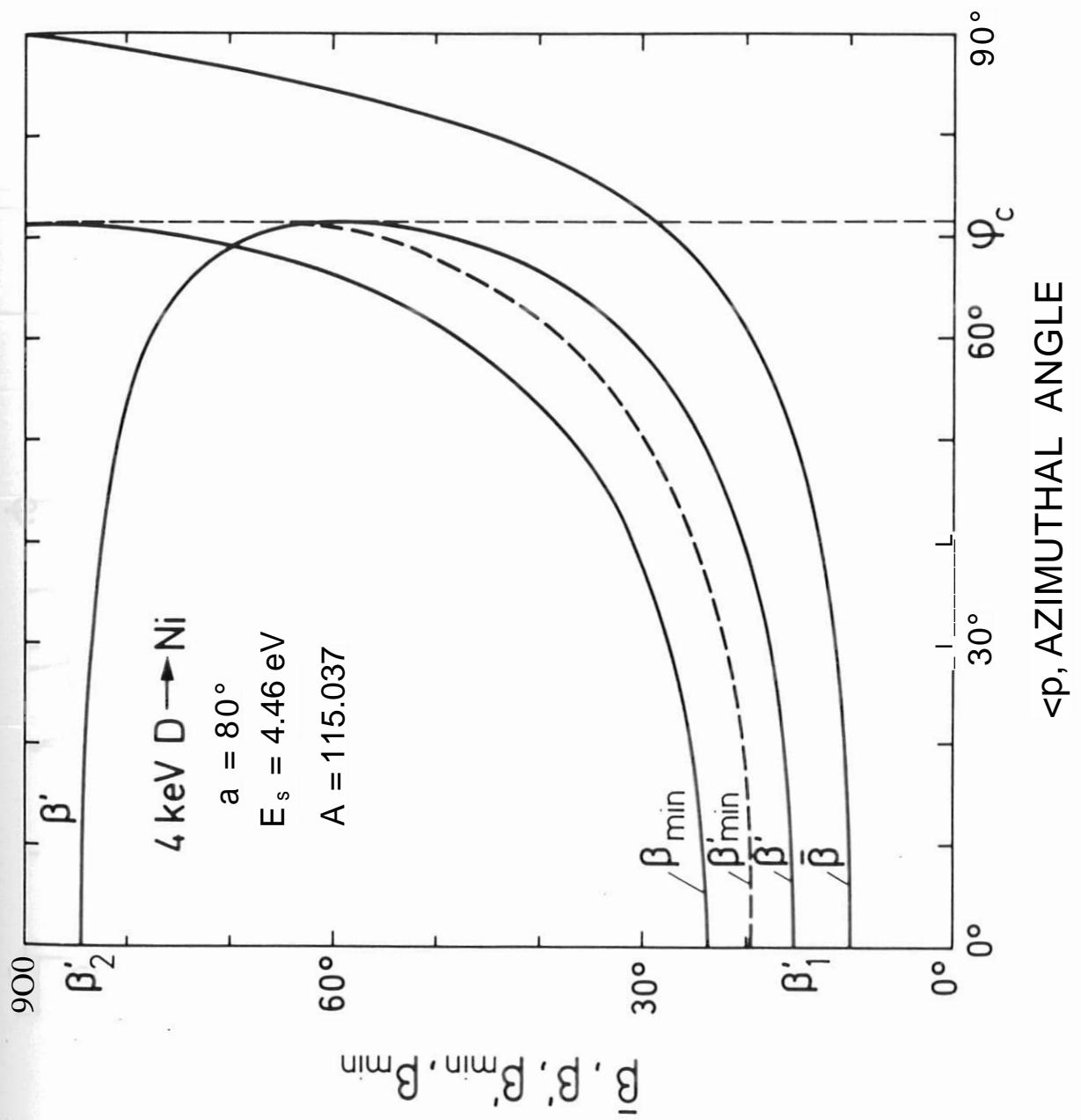


Fig. 35

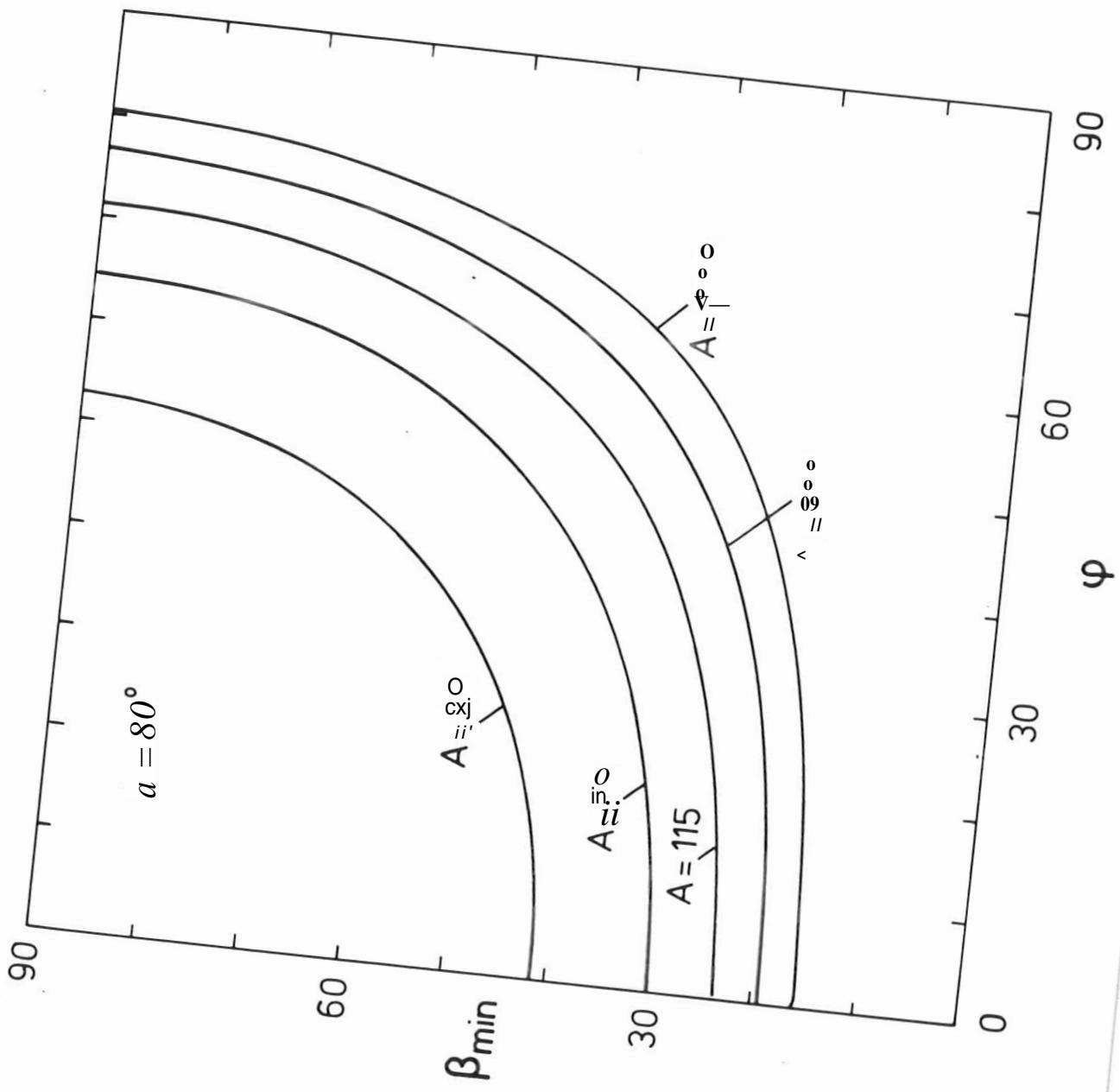


Fig. 9. 36

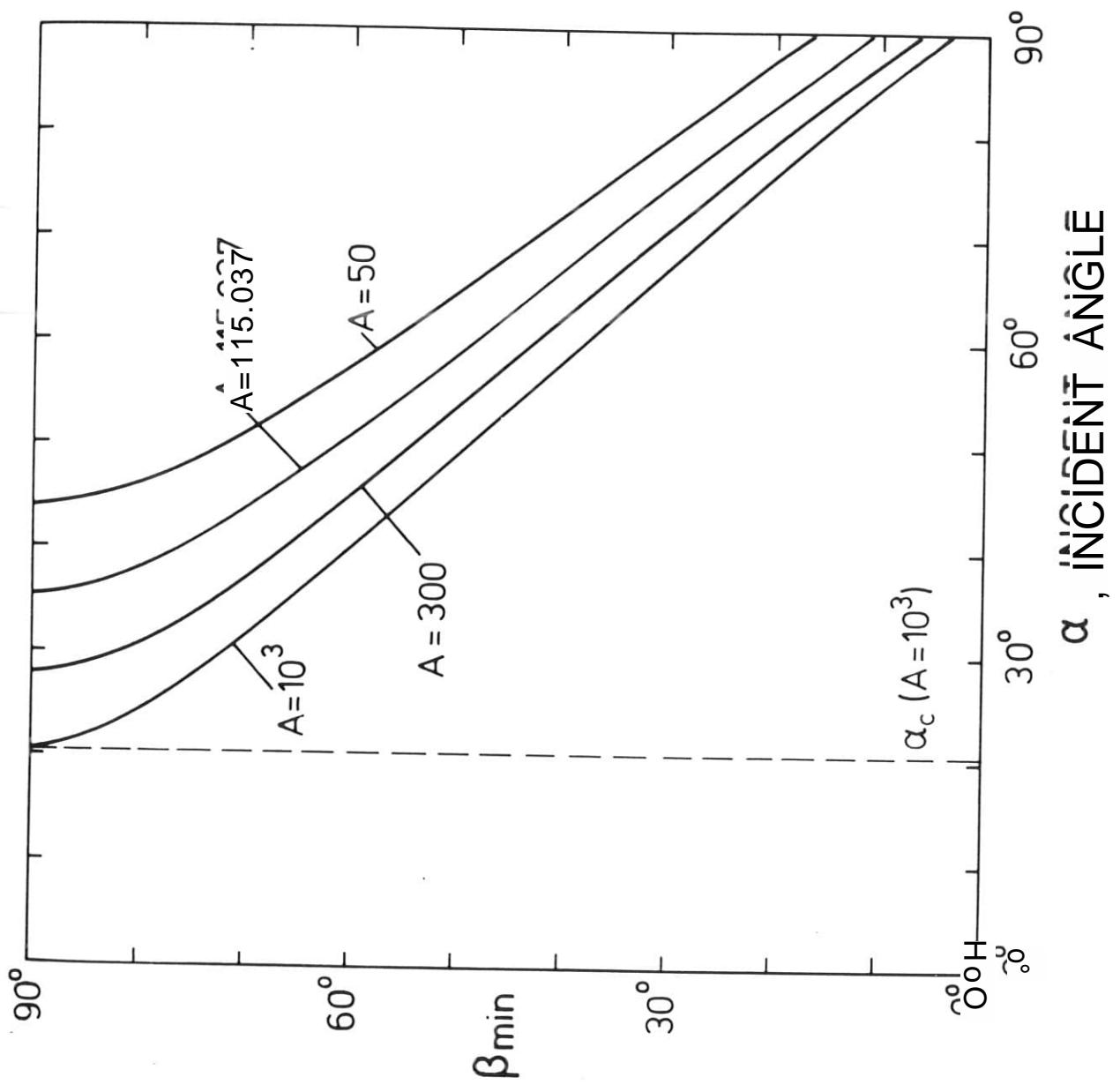


Fig. 37

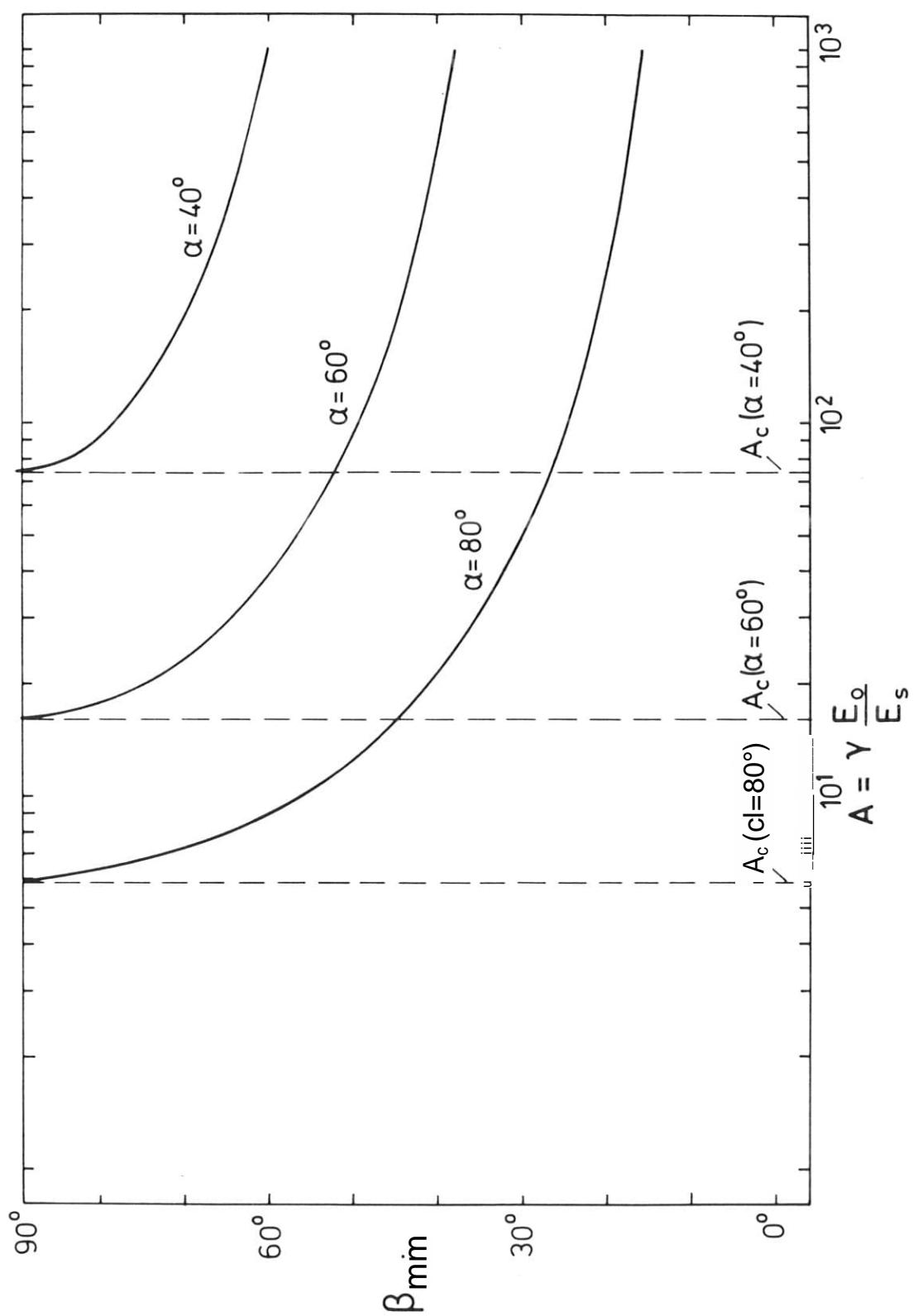


Fig. 38

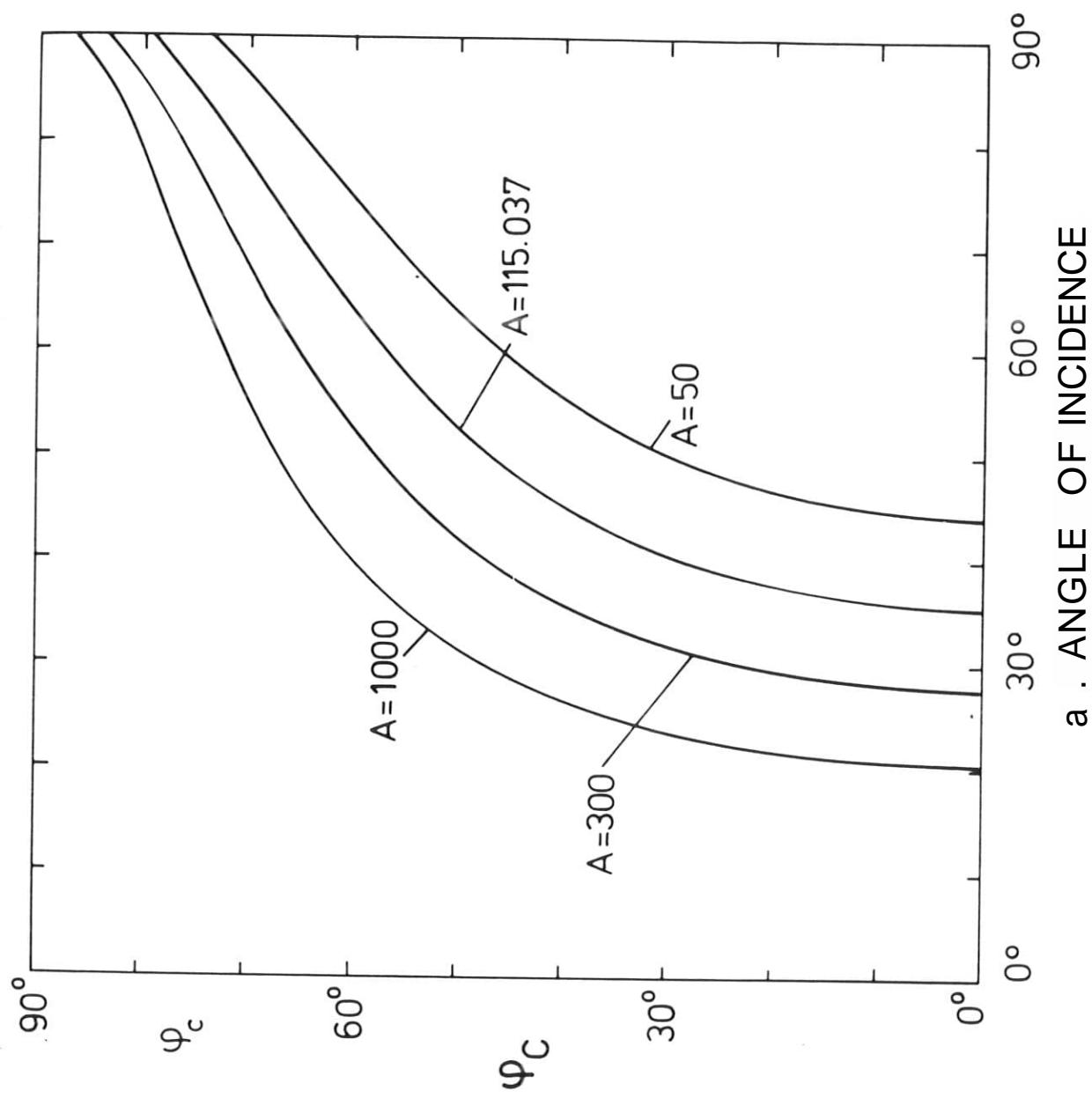


Fig. 39

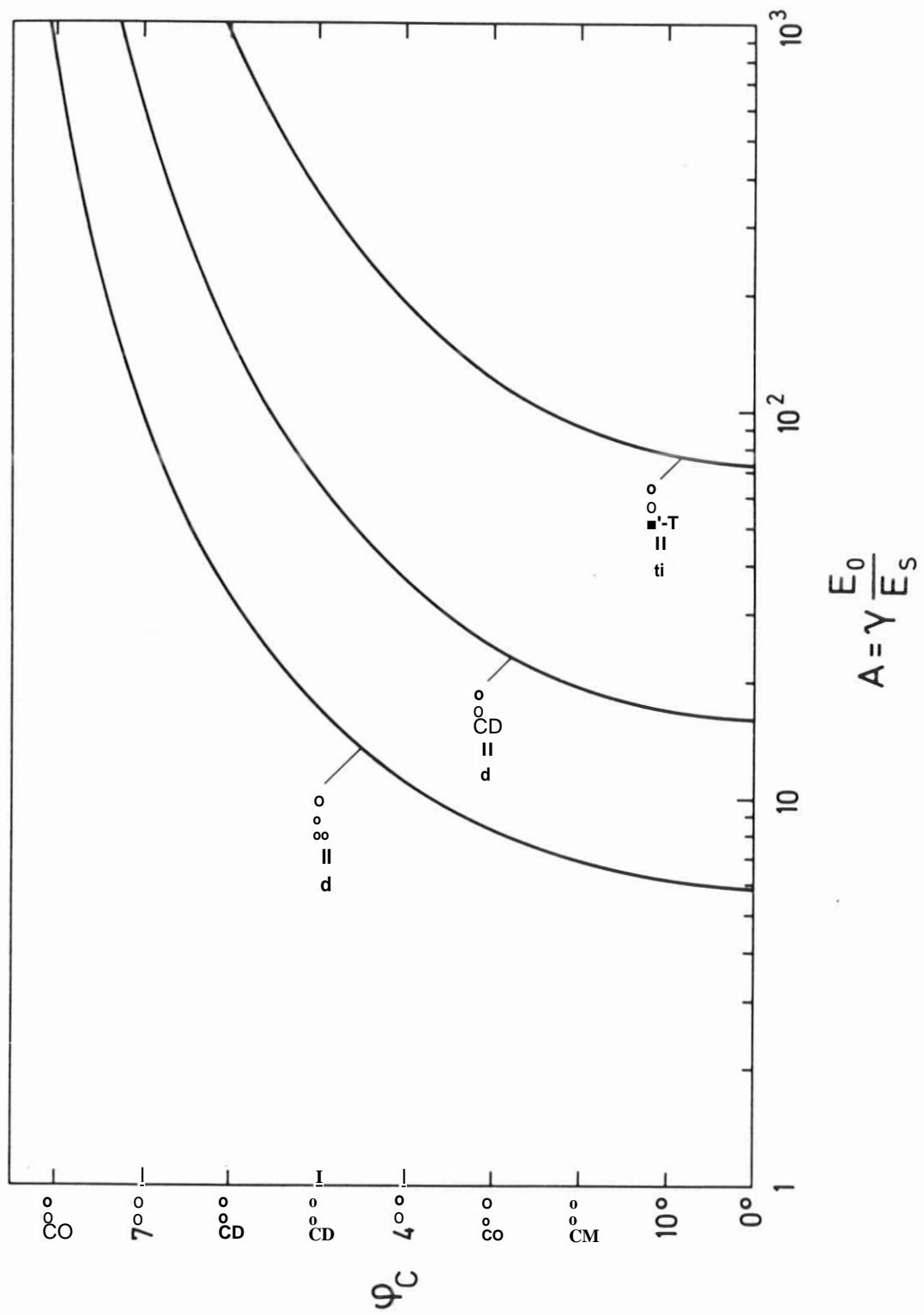


Fig. 40

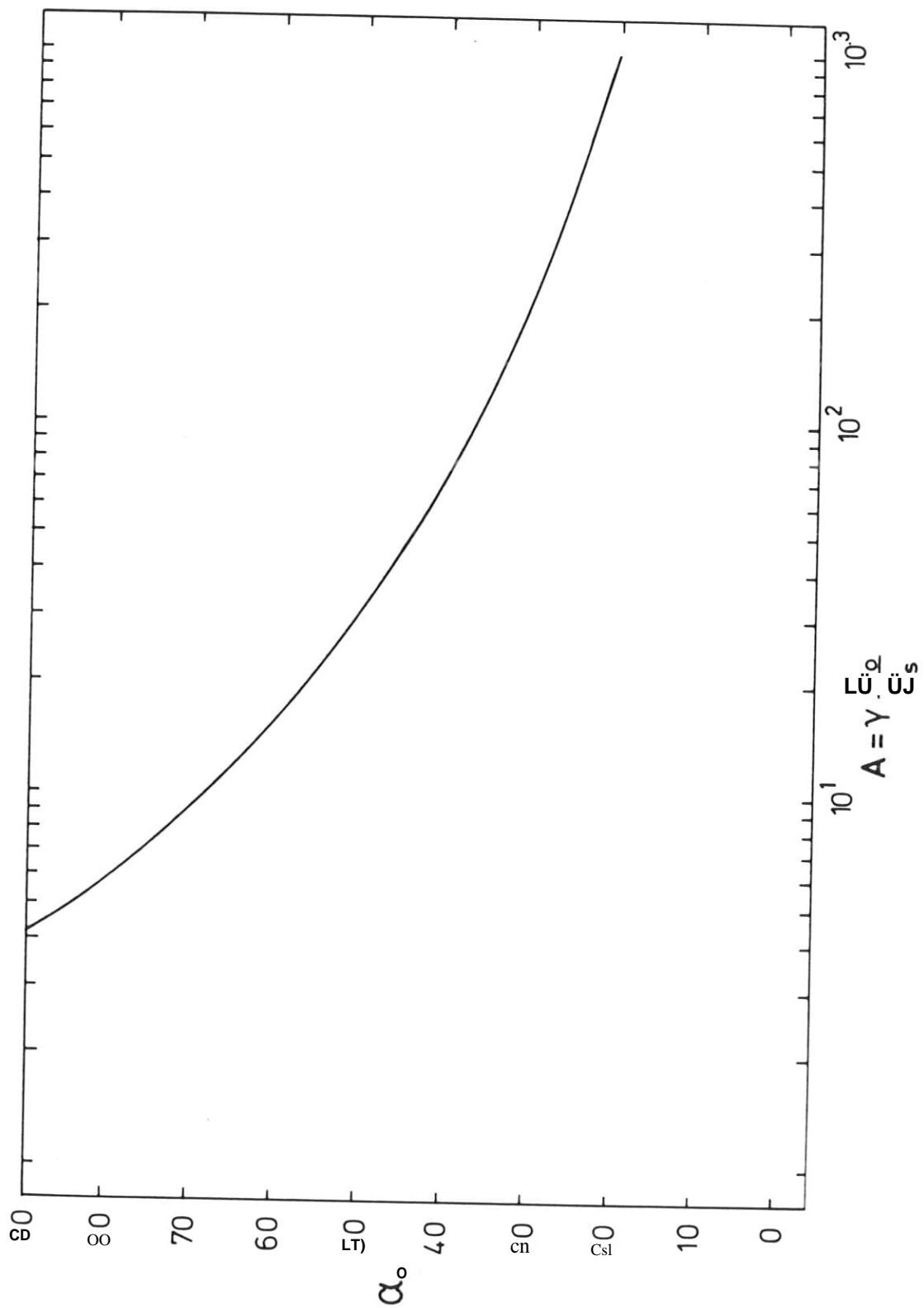


Fig . 41

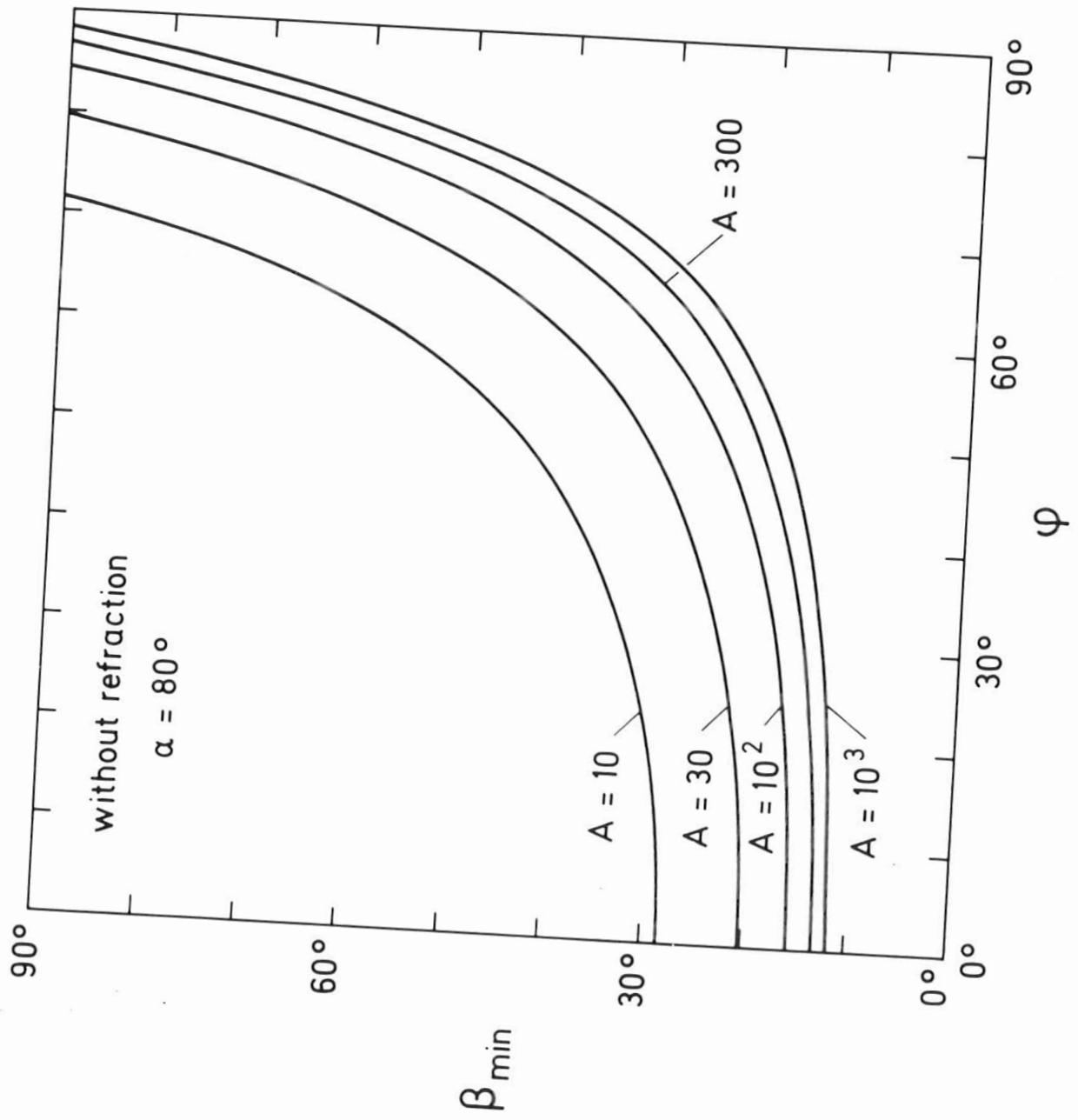


Fig. 42

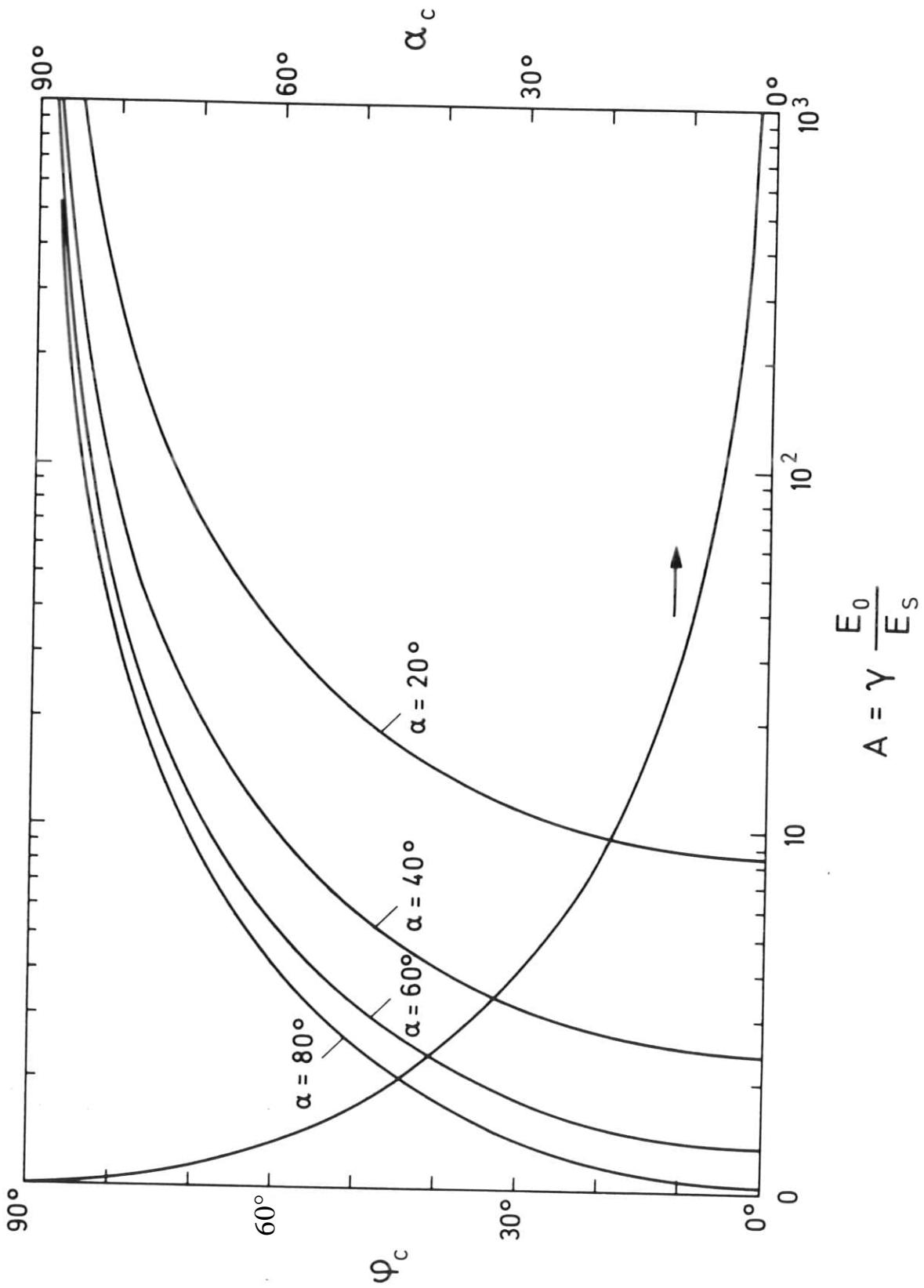


Fig. 43

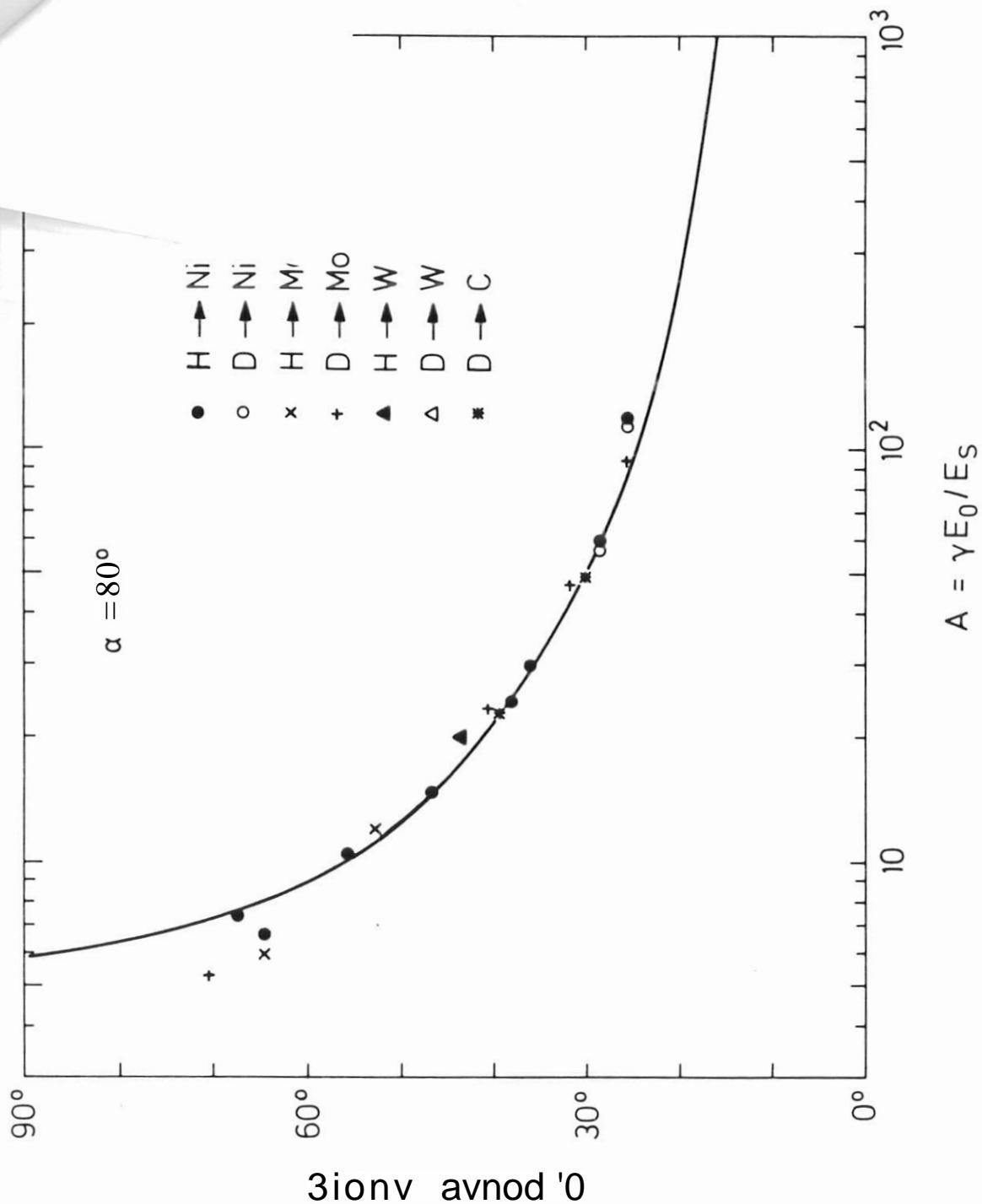
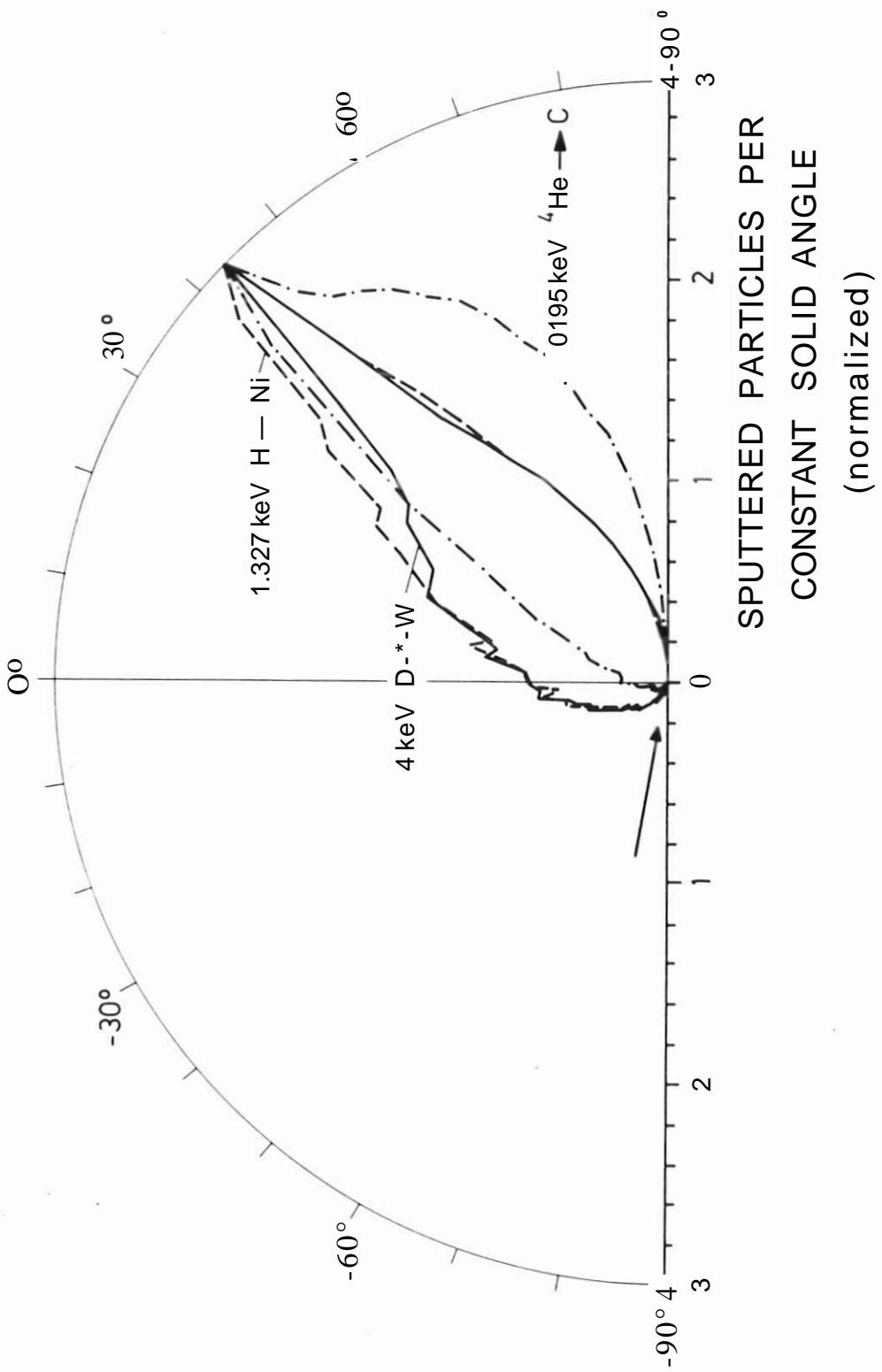


Fig. 44

$a = 80^\circ$



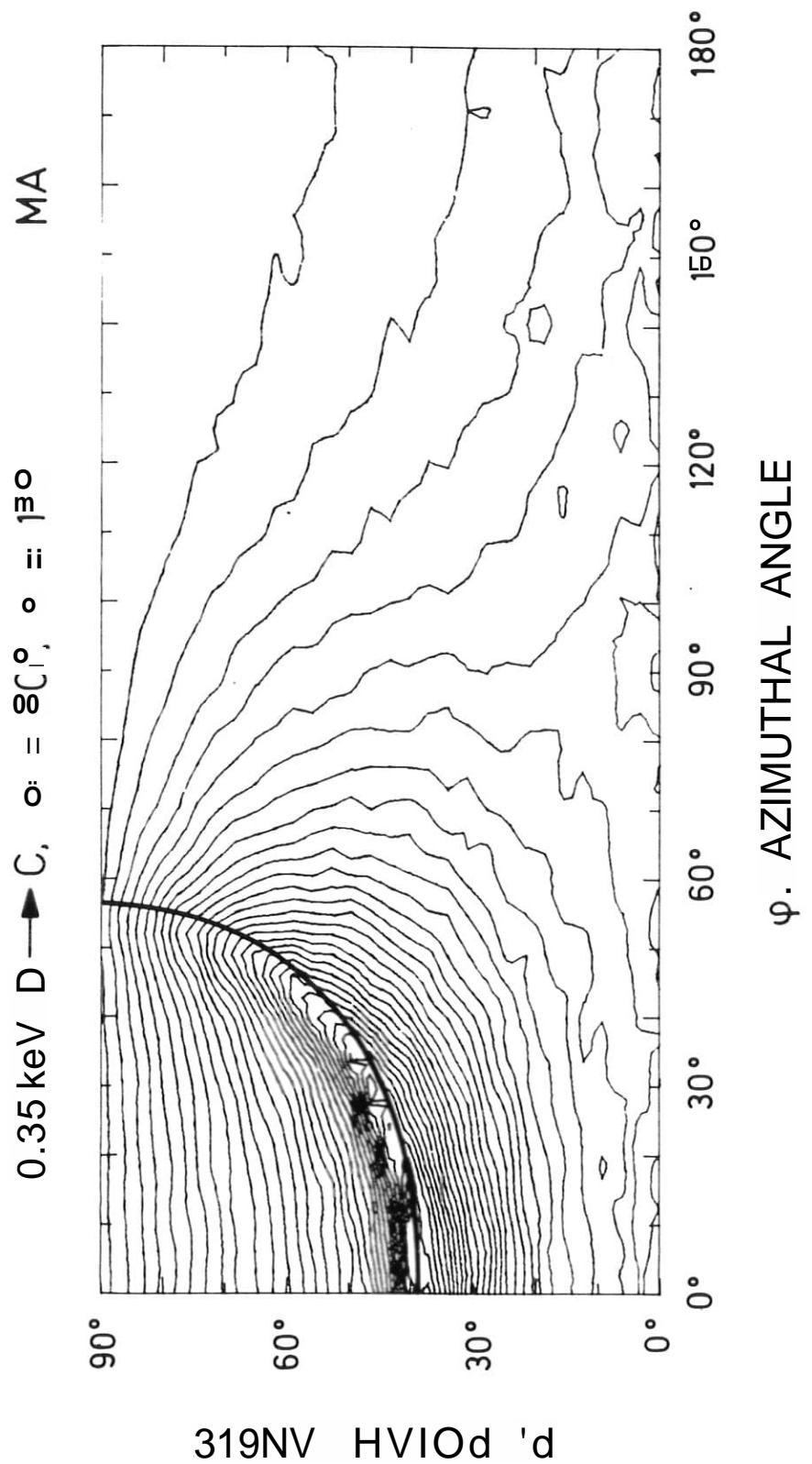
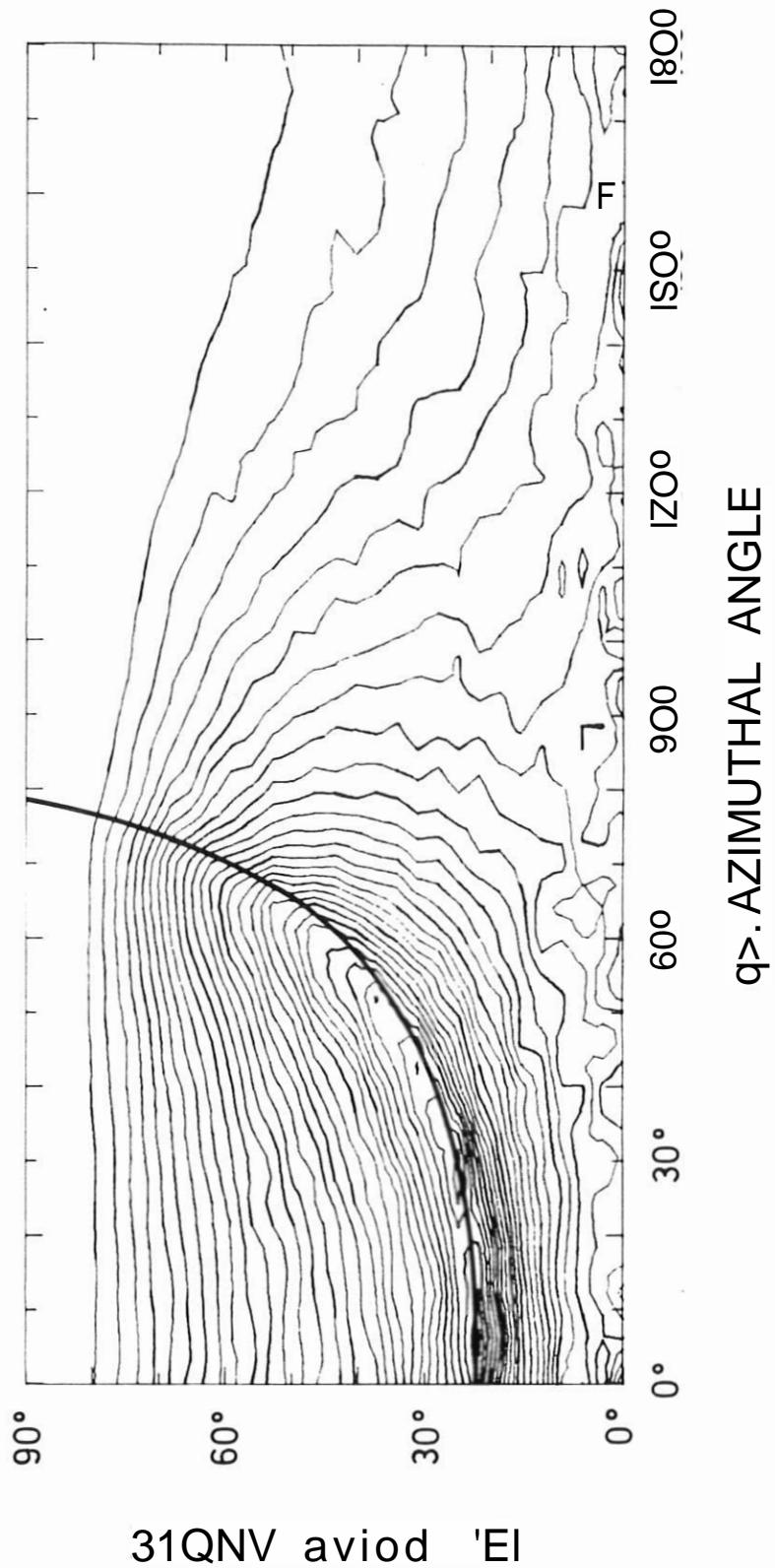


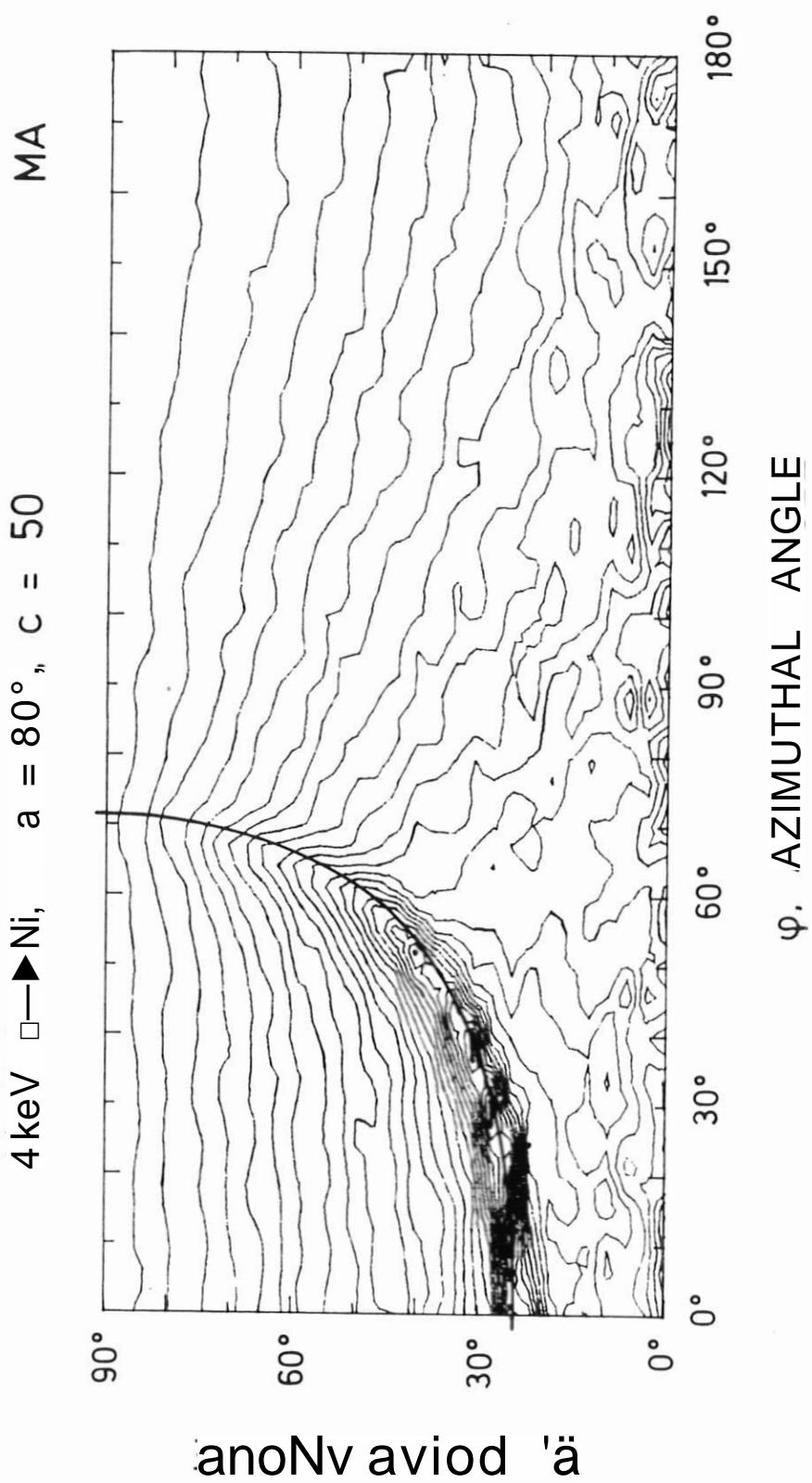
Fig. 46a

0.35keV D- C,  $\alpha = 80^\circ$ .  $C = 90$ , without refraction MA



31QNV aviod 'El

Fig. 4bb



anoNv aviod 'ä

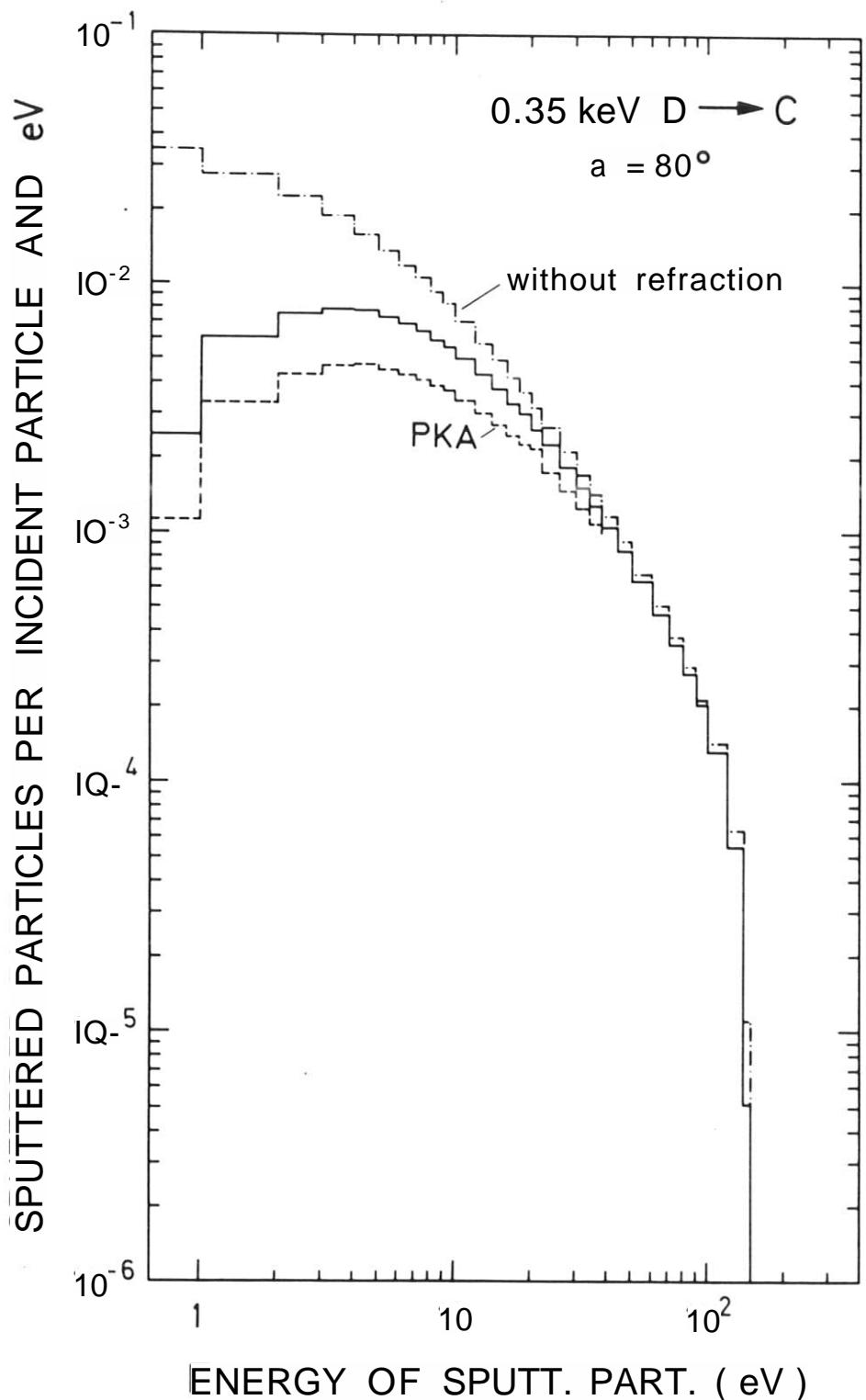


Fig. 48

SPUTT. PART PER eV, INCIDENT PART. AND AZIMUTHAL ANGULAR INTERVAL.

0.35 keV D  $\rightarrow$  C ,  $a = 80^\circ$

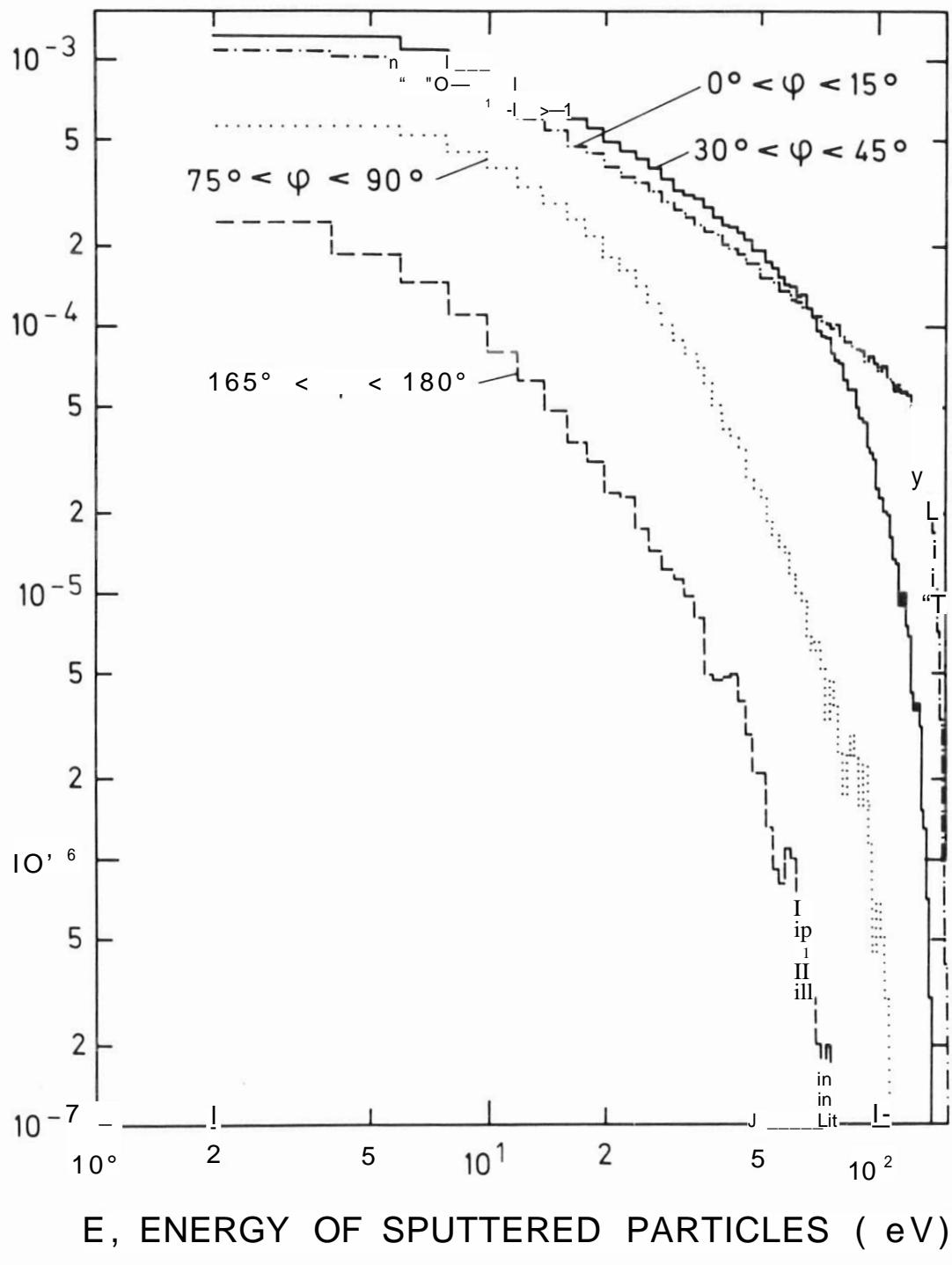


Fig. 49

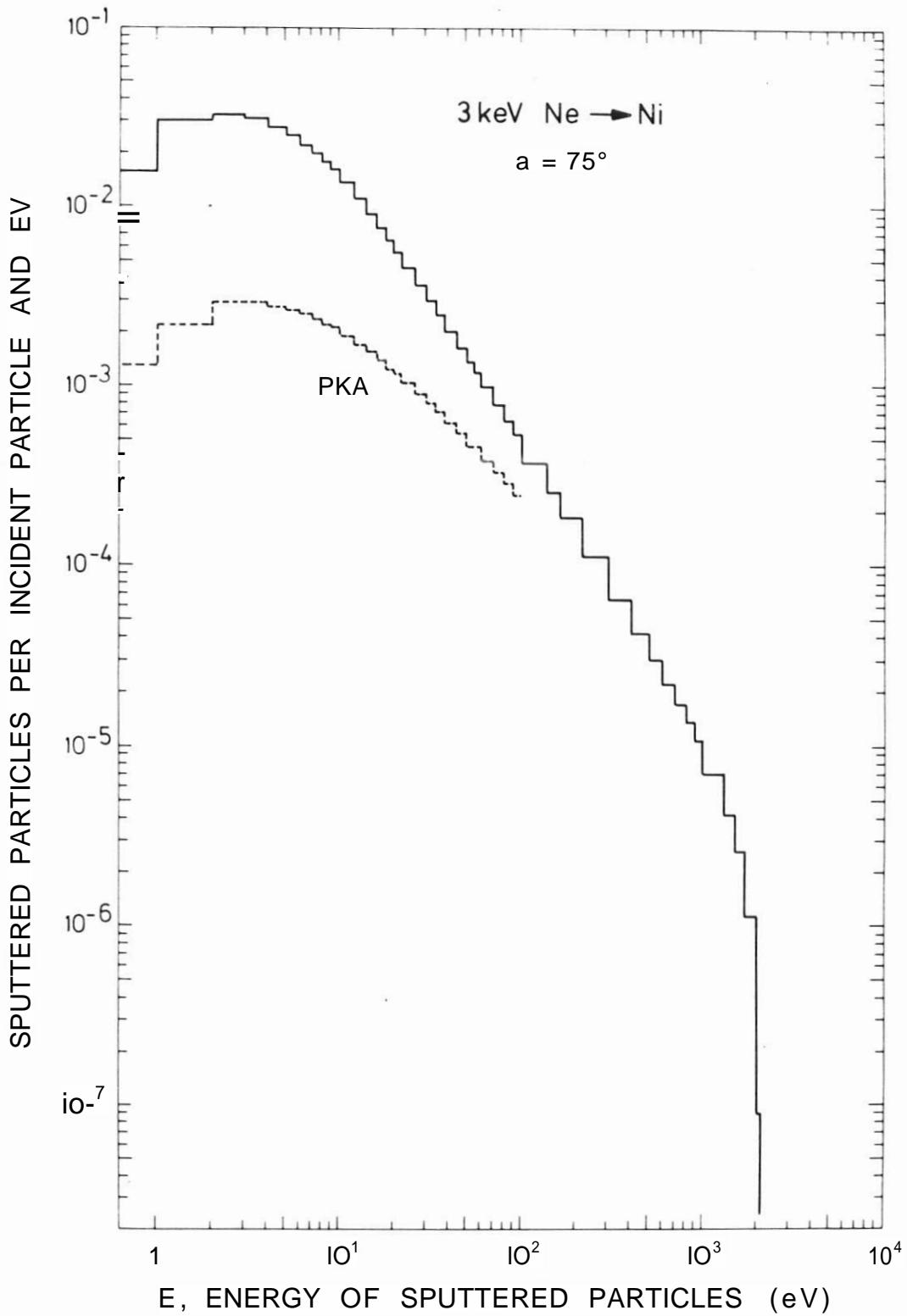


Fig. 50

SPUTT. PART. PER eV, INCIDENT PART. AND AZIMUTHAL ANGULAR INTERVAL.

3 keV Ne  $\rightarrow$  Ni  $\alpha = 75^\circ$

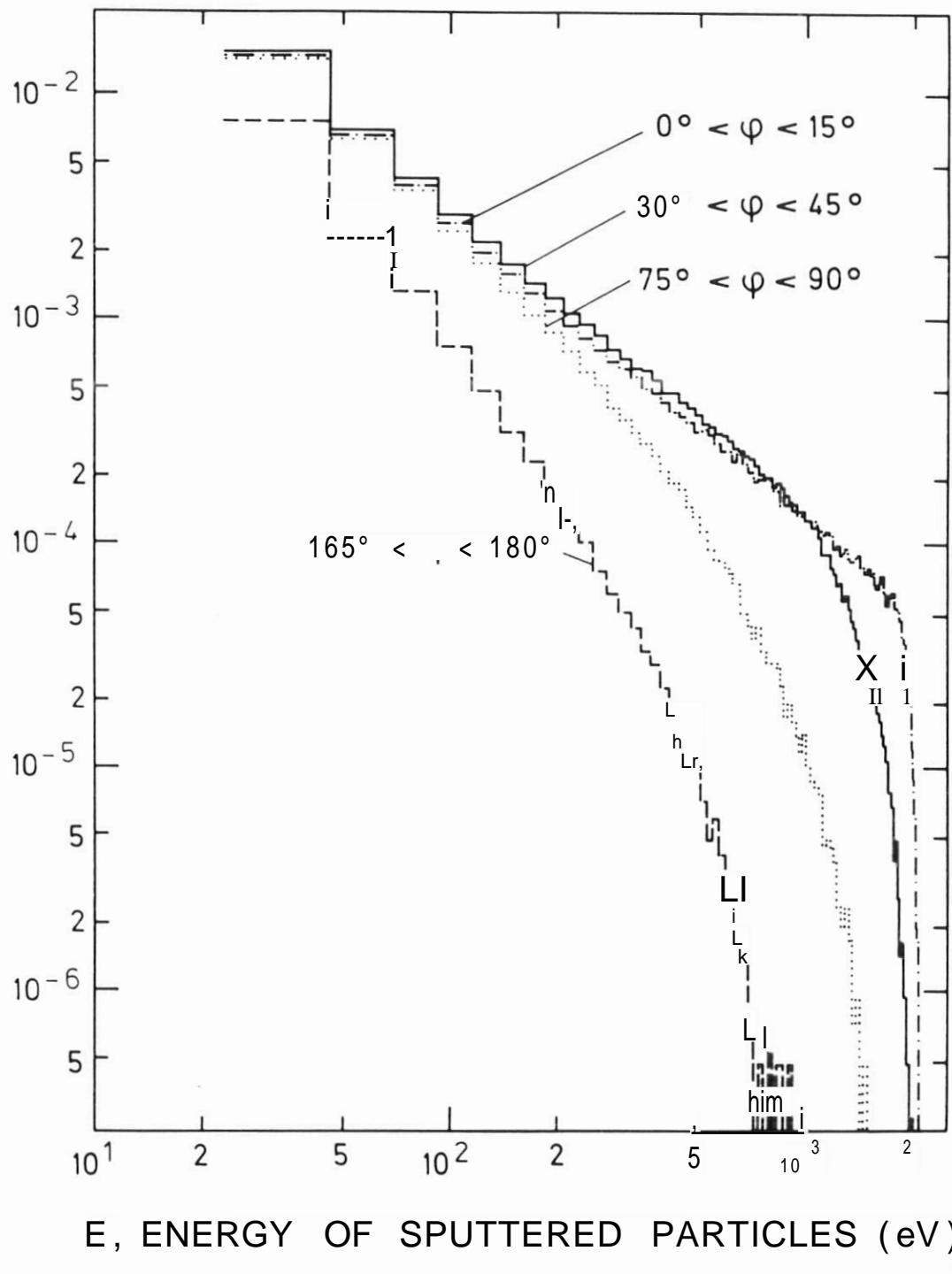
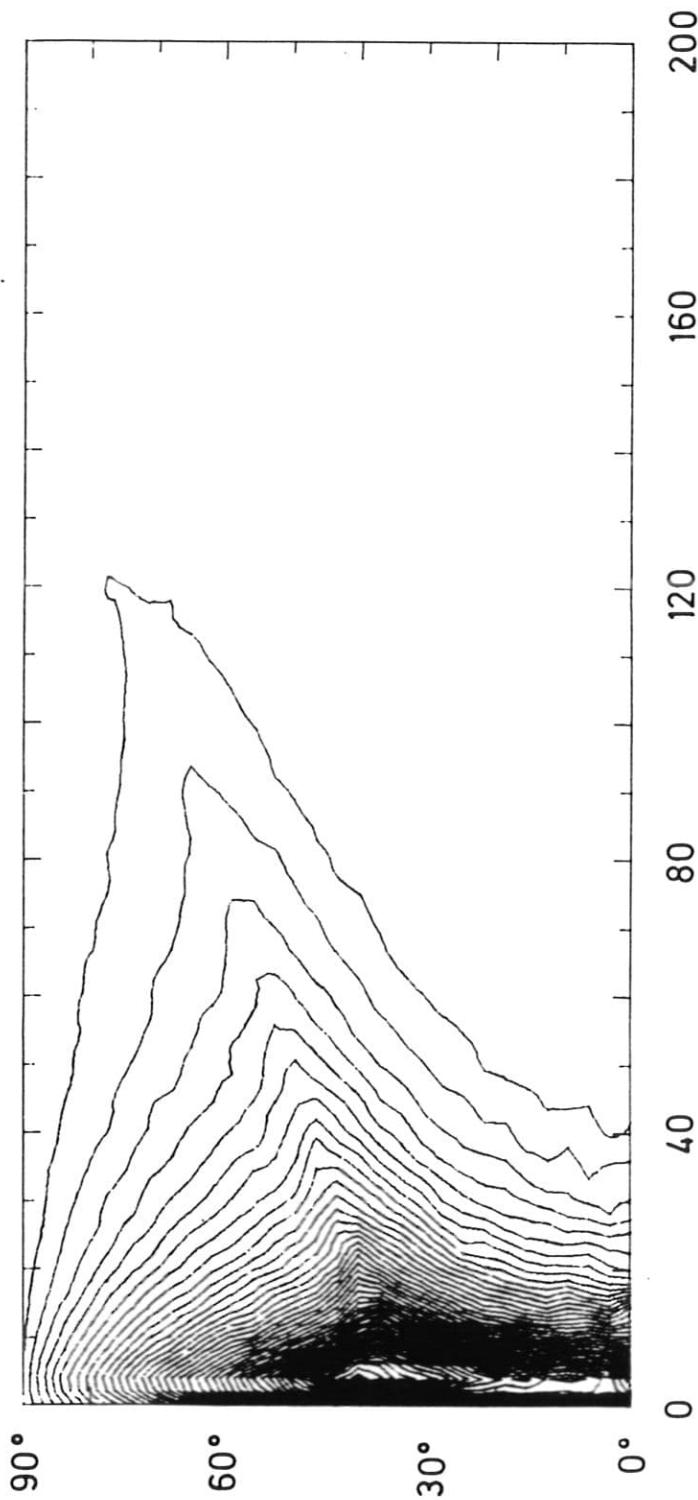


Fig. 51

0 35 keV D—► C,  $\alpha = 80^\circ$ , INTEGRATED OVER  $q$ ,  $O = \frac{1}{D}O$



ENERGY OF SPUTTERED PARTICLES [eV]

310NV HVIOd '£)

Fig. 52a

0.35 keV D → C,  $\alpha = 80^\circ$ ,  $0^\circ < \varphi < 15^\circ$ ,  $C = 40$

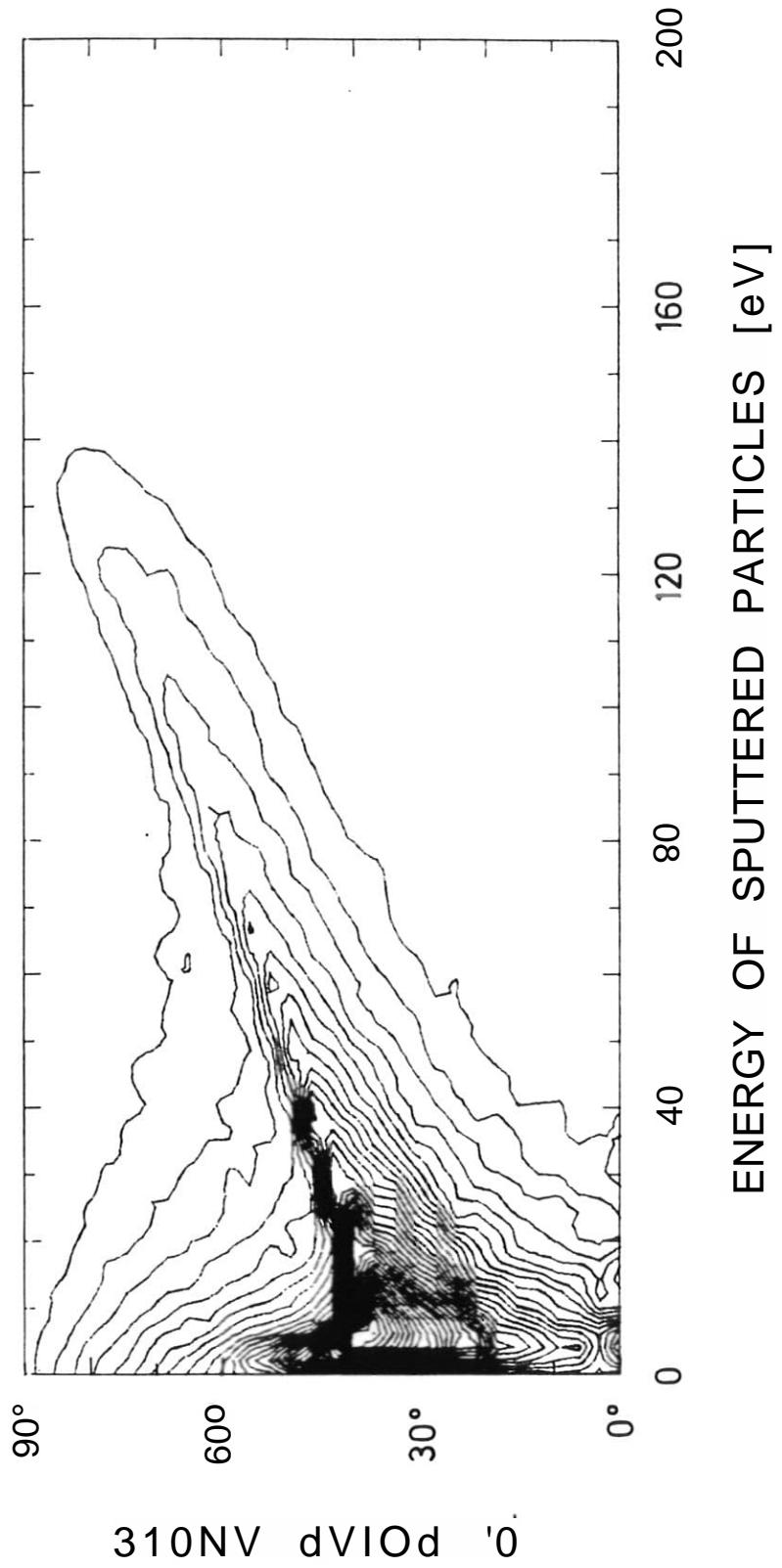
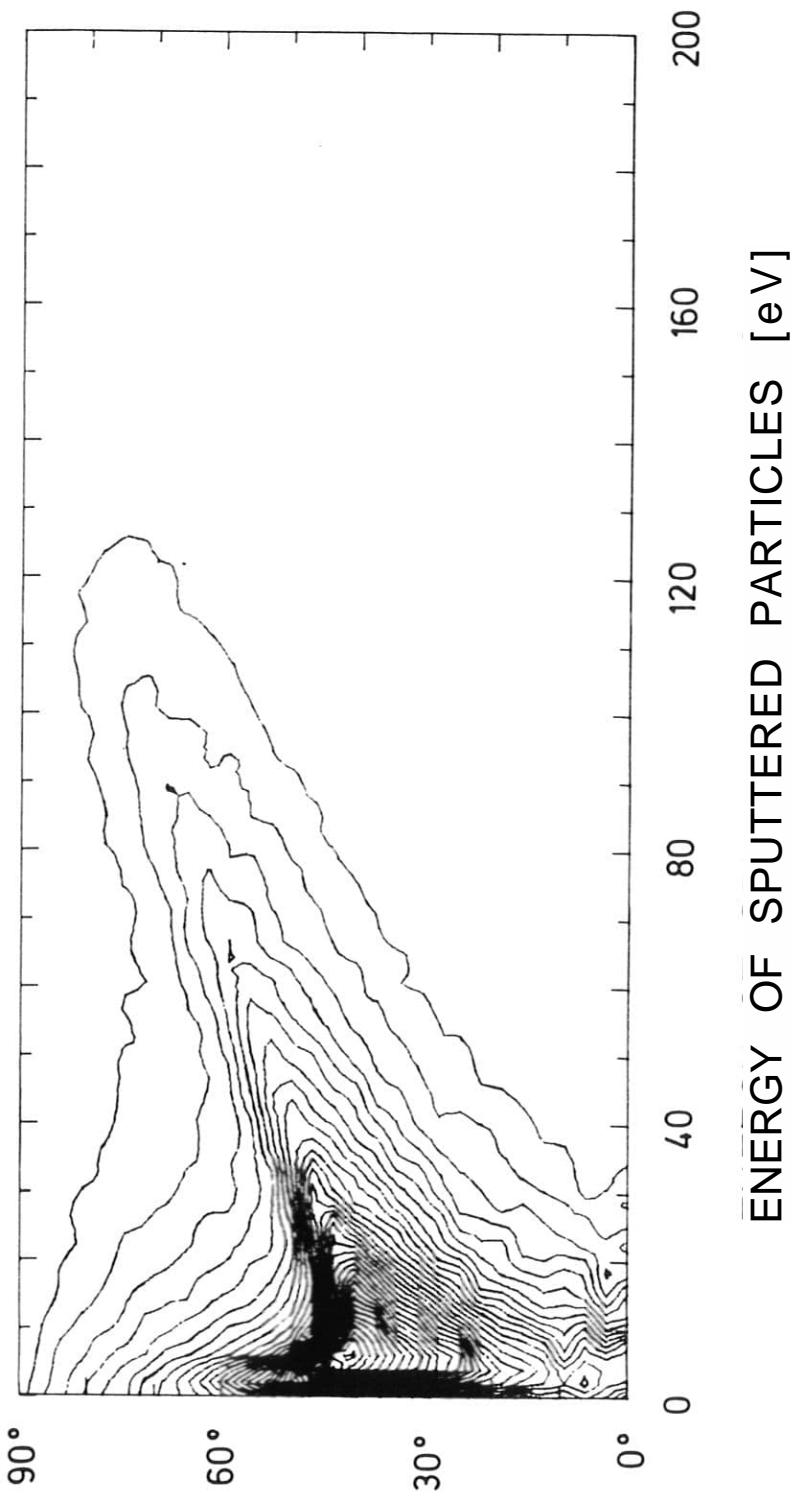


Fig. 52b

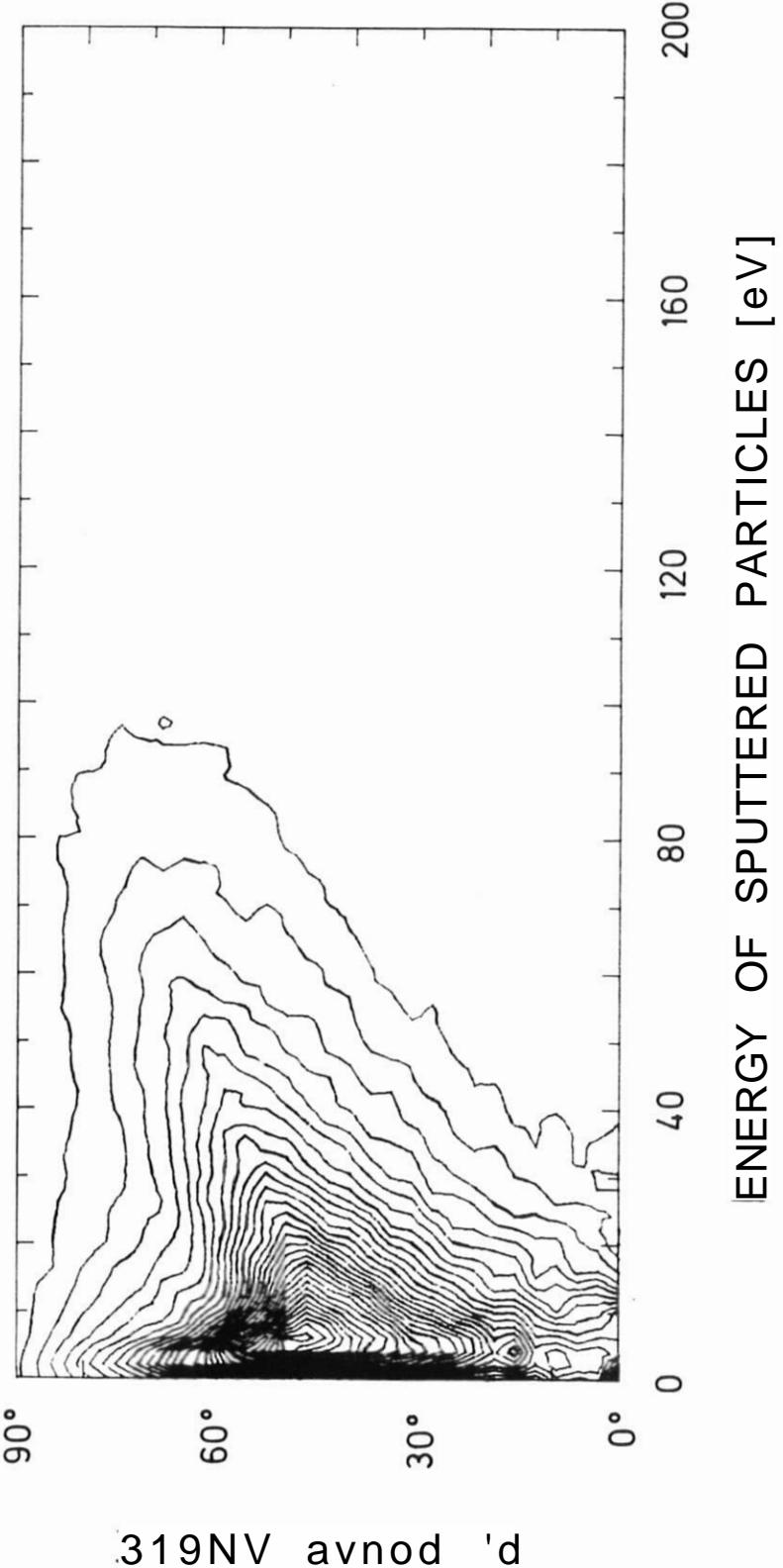
$0.35 \text{ keV}$   $\bar{D} - \bar{C}$ ,  $a = 80^\circ$ ,  $15^\circ < \langle p \rangle < 30^\circ$ ,  $C = 40$



319NV aviod 'd

Fig. 52c

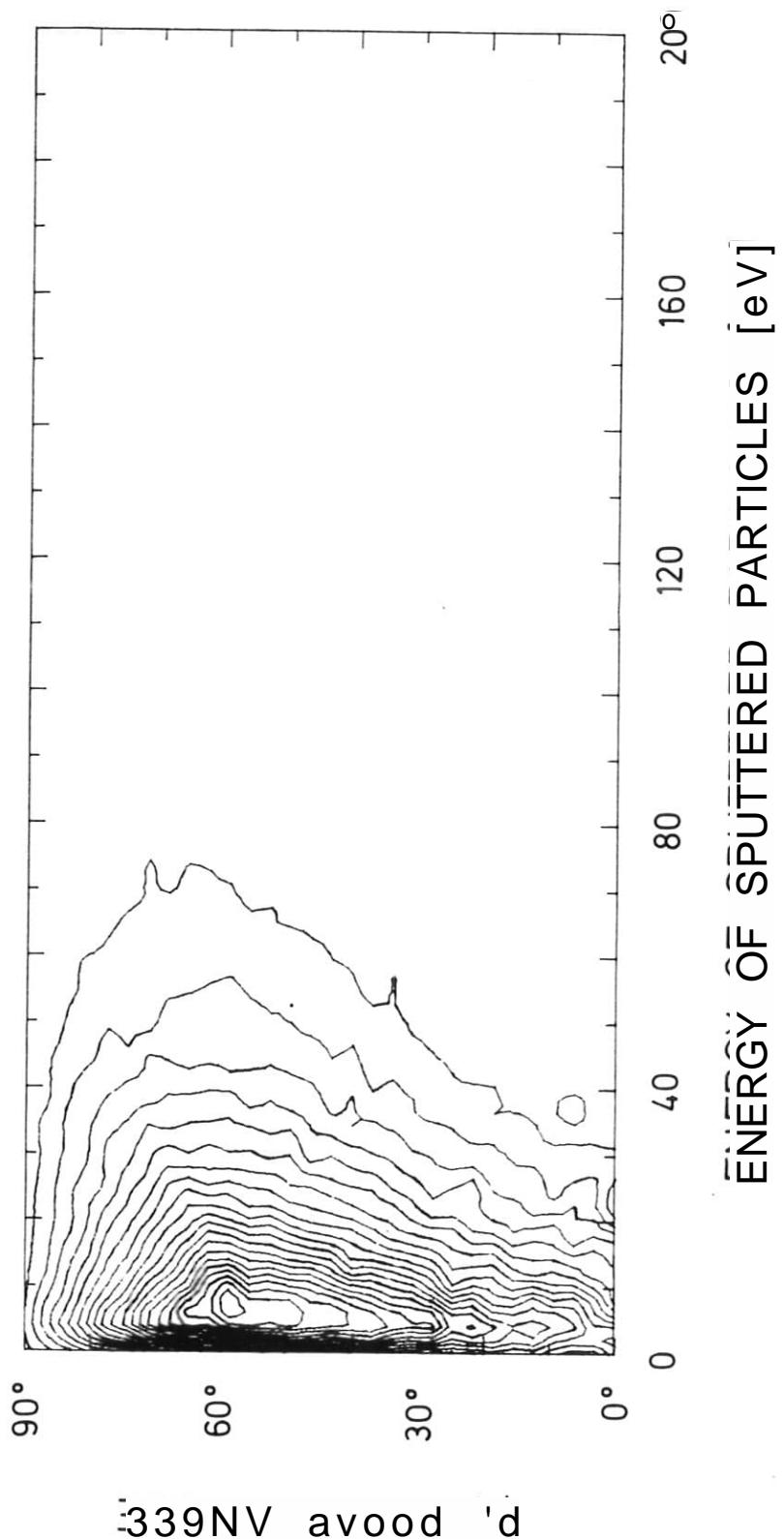
0.35 keV D → C.  $\alpha = 80^\circ$ ,  $30^\circ < q < 45^\circ$ ,  $C = 40$



319NV avnod 'd

Fig. S2d

$\hat{0.35}$  keV  $\bar{D} \rightarrow \bar{C}$ ,  $a = 80^\circ$ ,  $45^\circ < \varphi < 45^\circ_*$ ,  $C = 40$



339NV avood 'd

Fig. 52e

0.35 keV D  $\rightarrow$  C,  $\alpha = 80^\circ$ ,  $60^\circ < \varphi < 75^\circ$ ,  $c = 40$

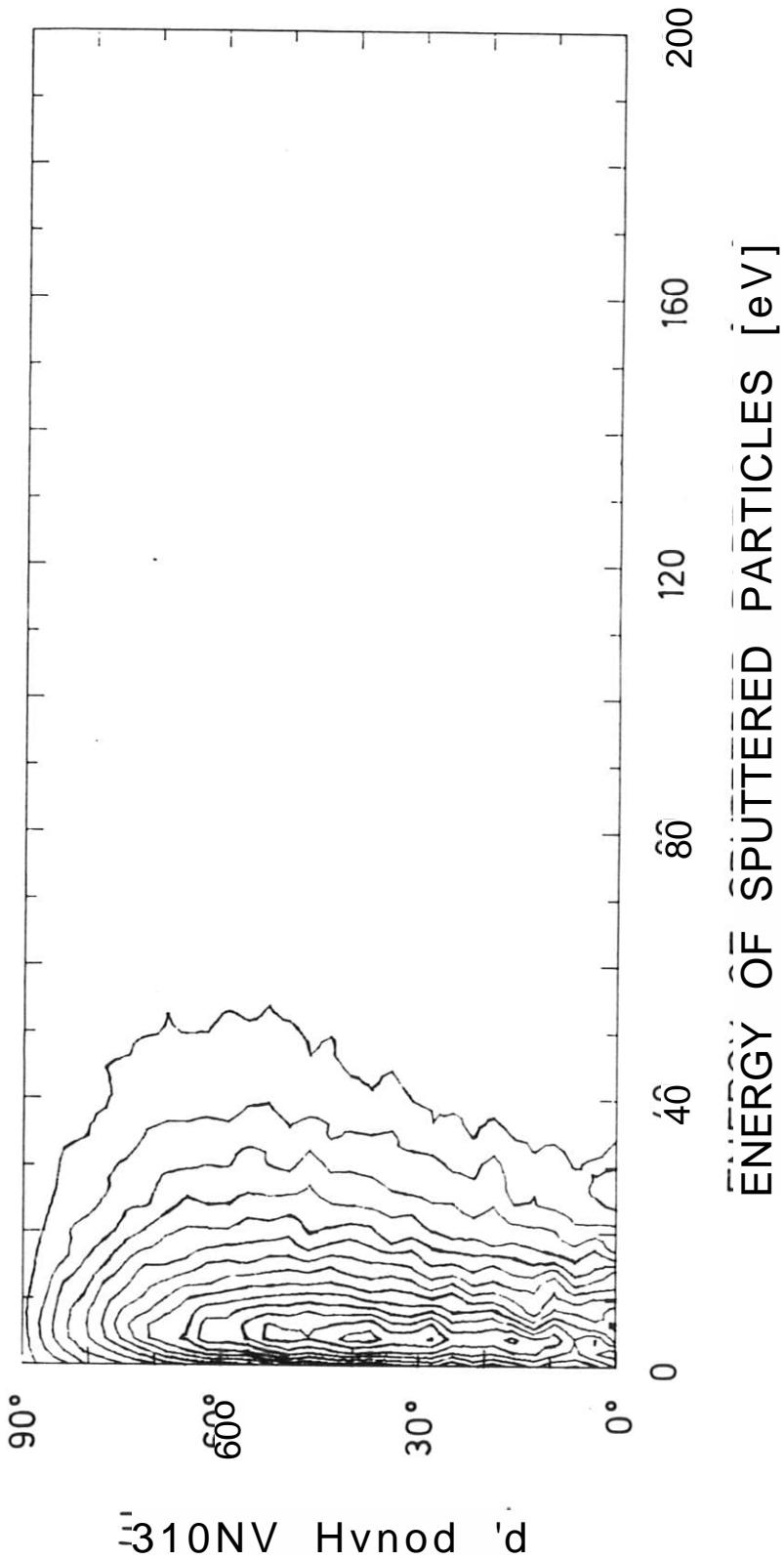


Fig. 52f

ENERGY OF SPUTTERED PARTICLES [eV]

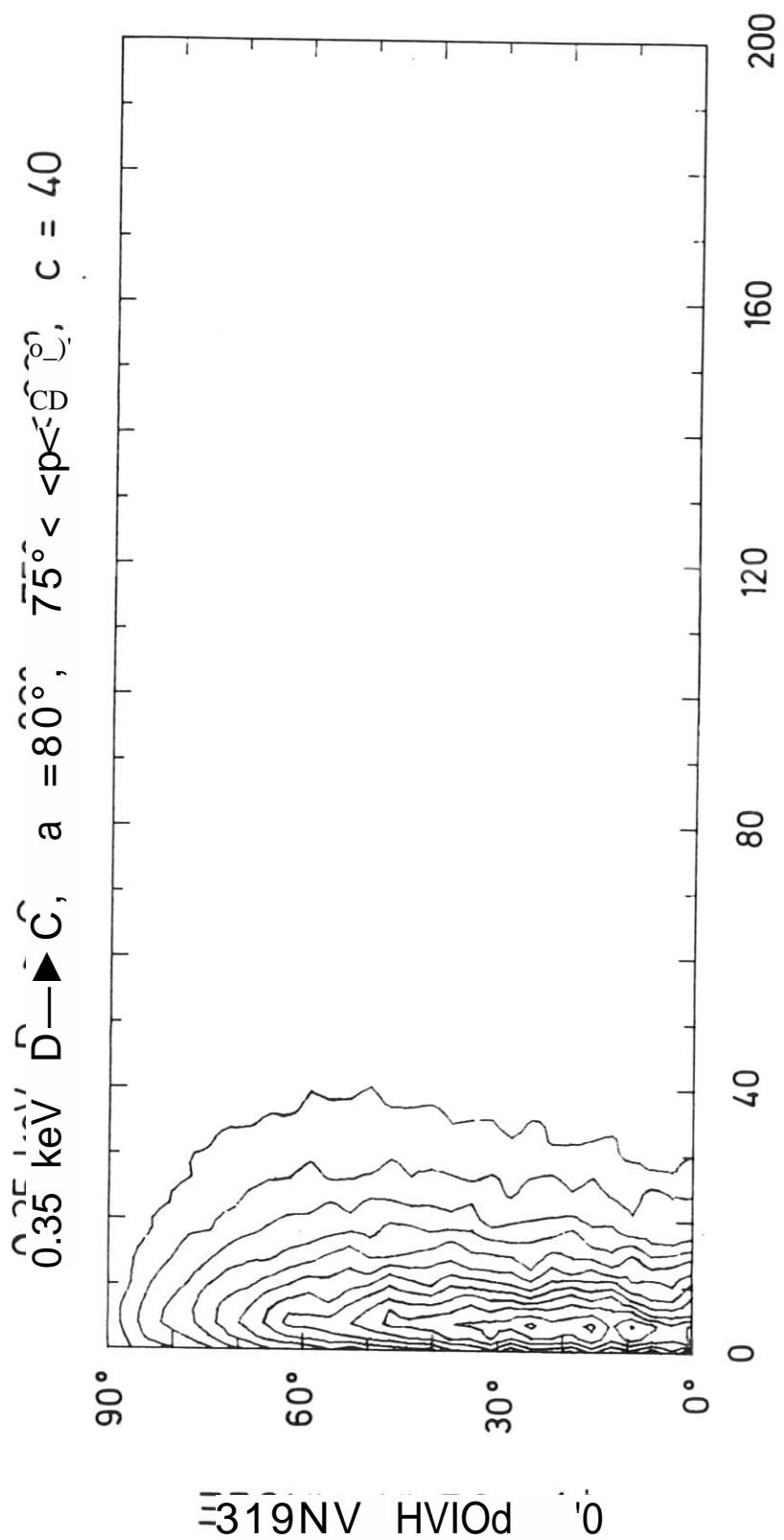


Fig. 52g

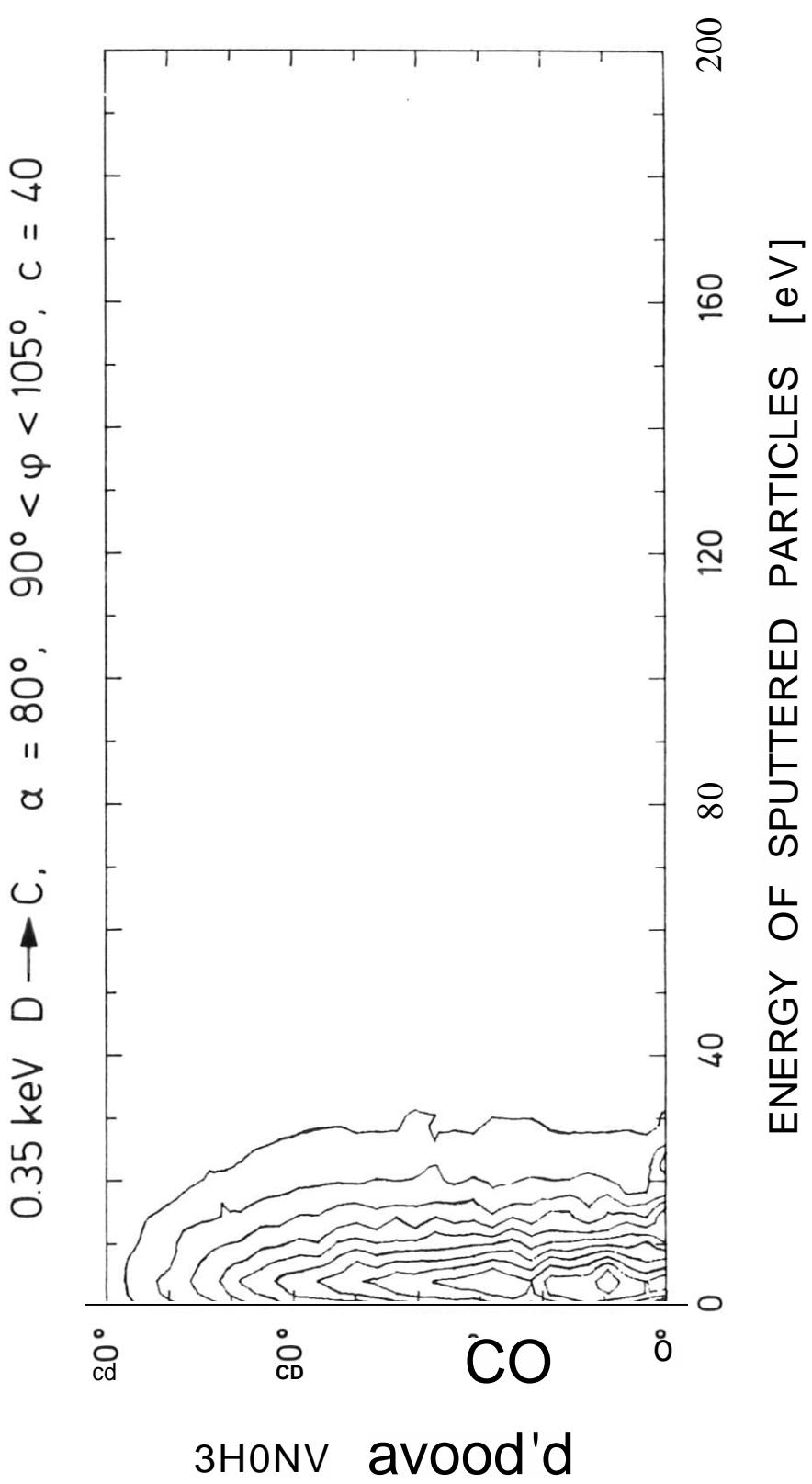


Fig. 52h

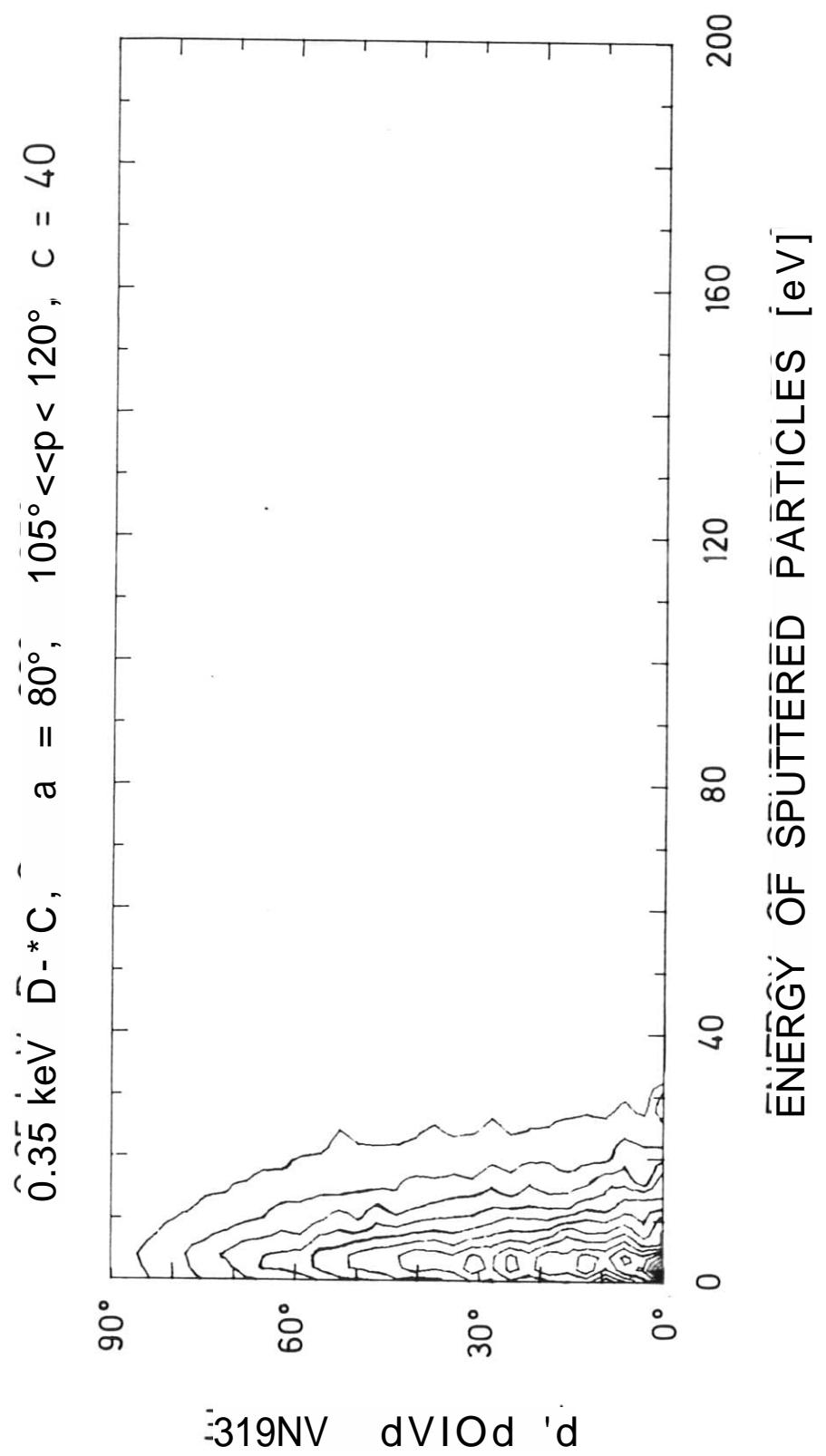


Fig. 52i

$0.35 \text{ keV } D \rightarrow C, \alpha = 80^\circ, 120^\circ < \theta < 135^\circ, c = 40$

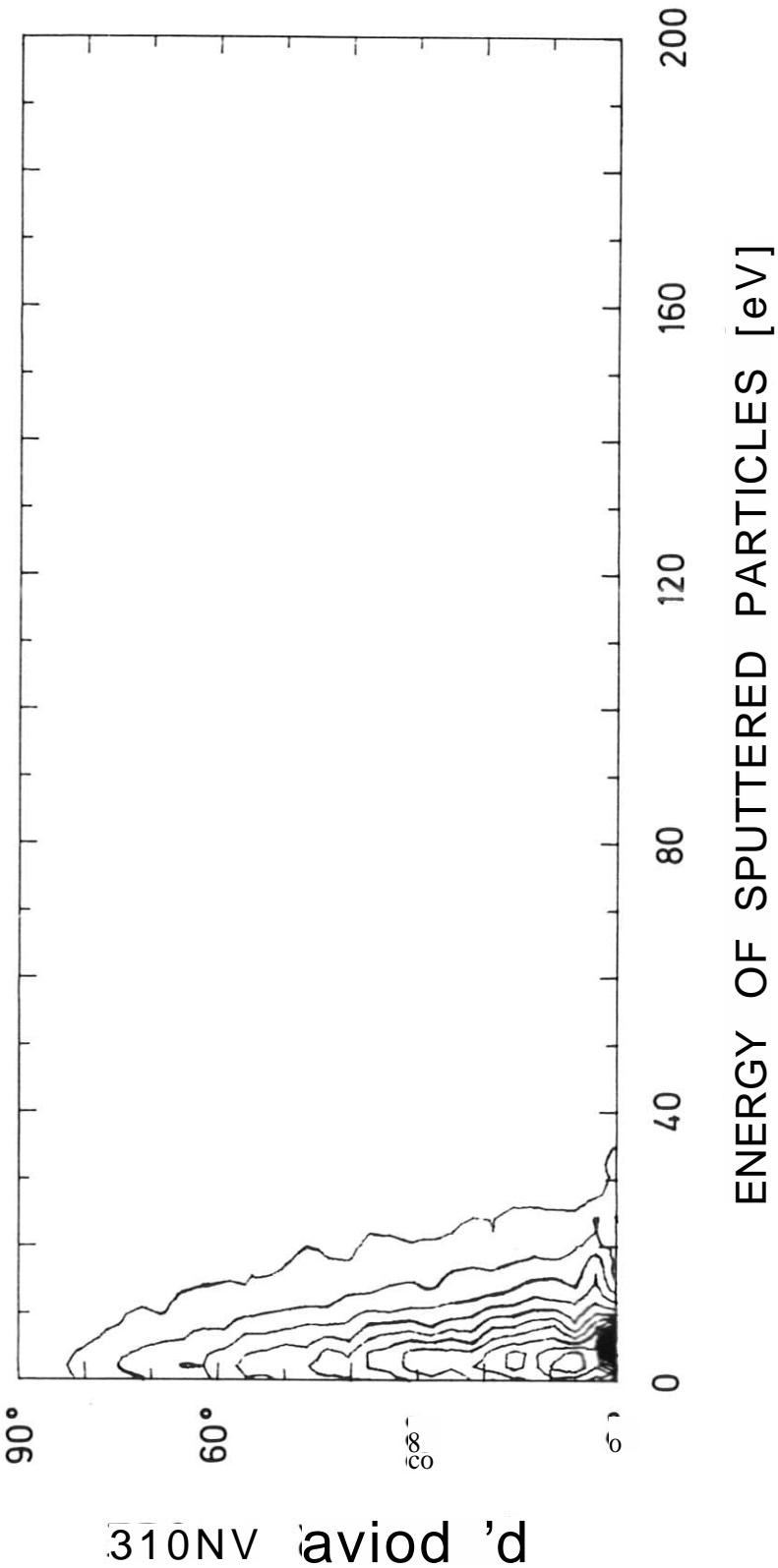


Fig. 52j

0.35 keV D-\*C,       $\alpha = 80^\circ$ ,       $135^\circ < \theta < 150^\circ$ ,  $C = 40$

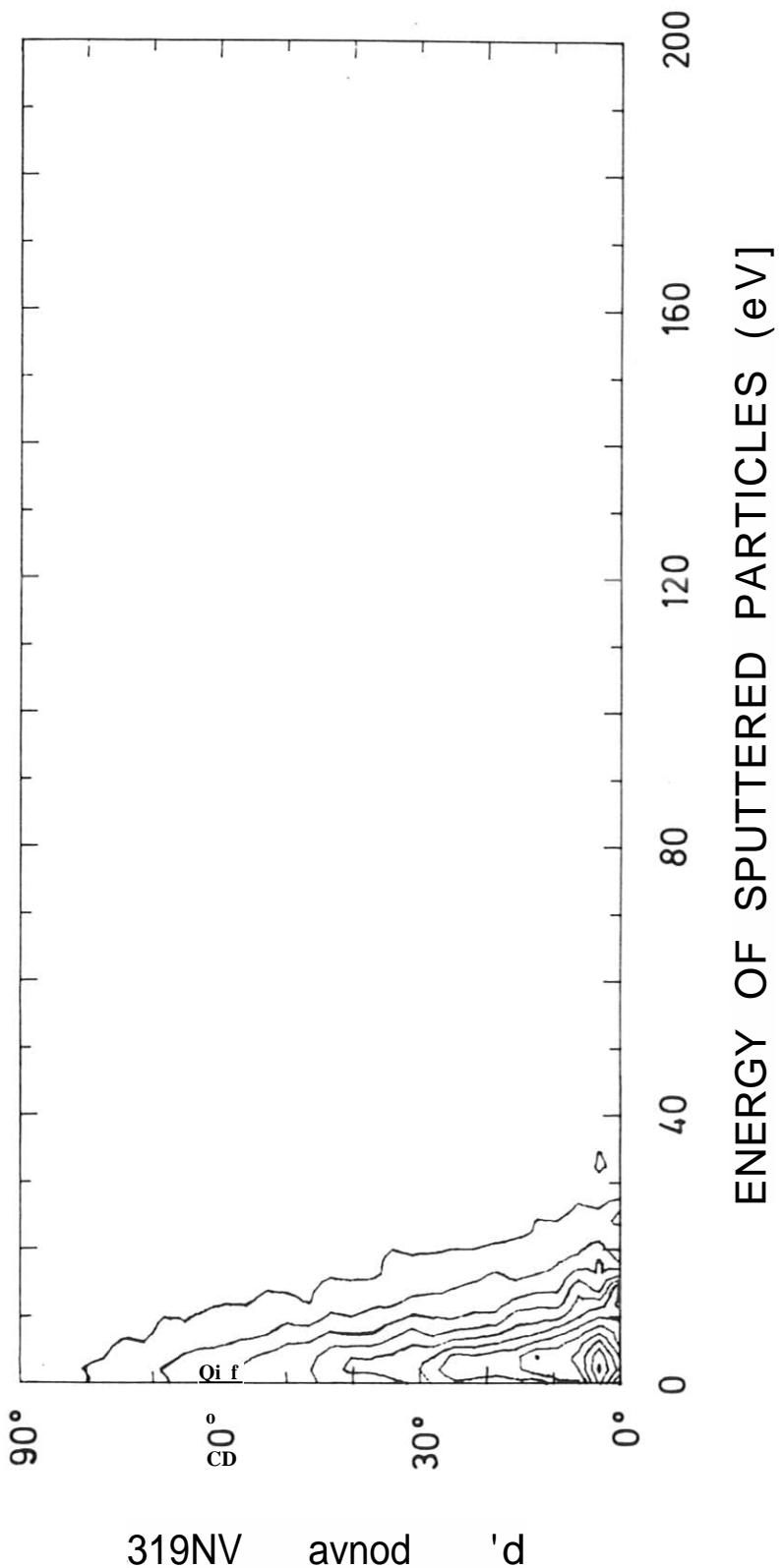


Fig. 52k

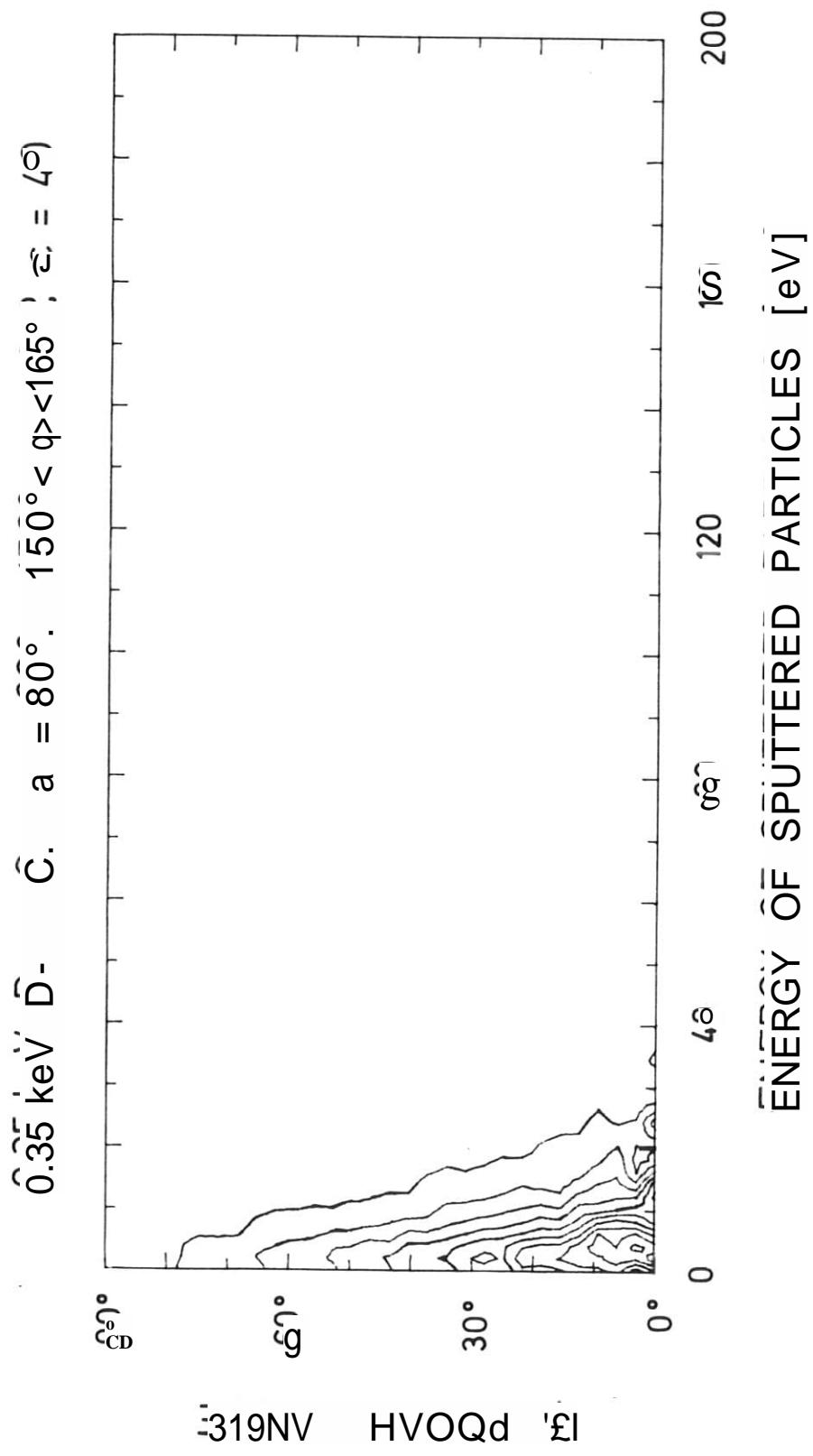


Fig. 521

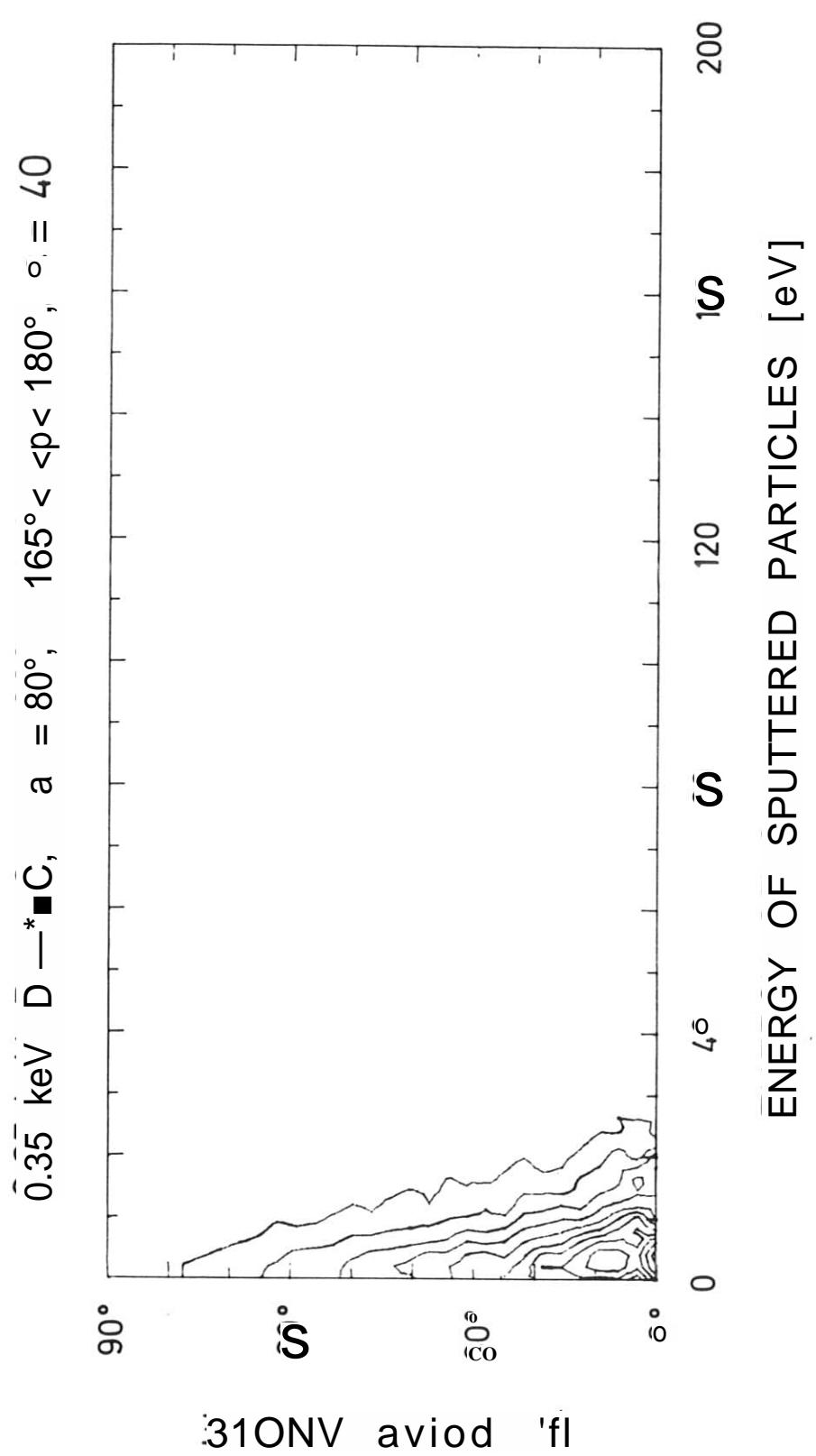


Fig. 52n

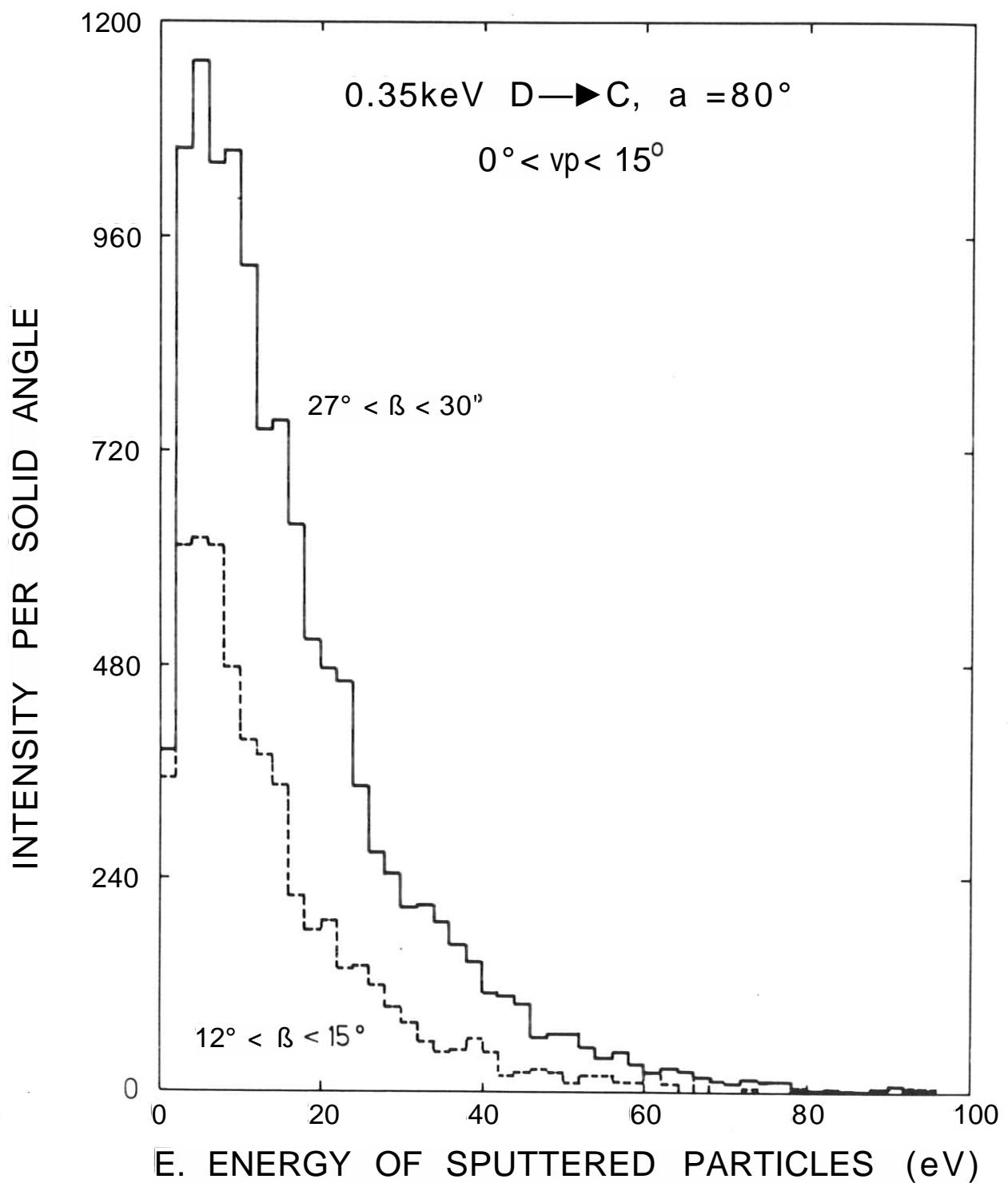


Fig. 53a

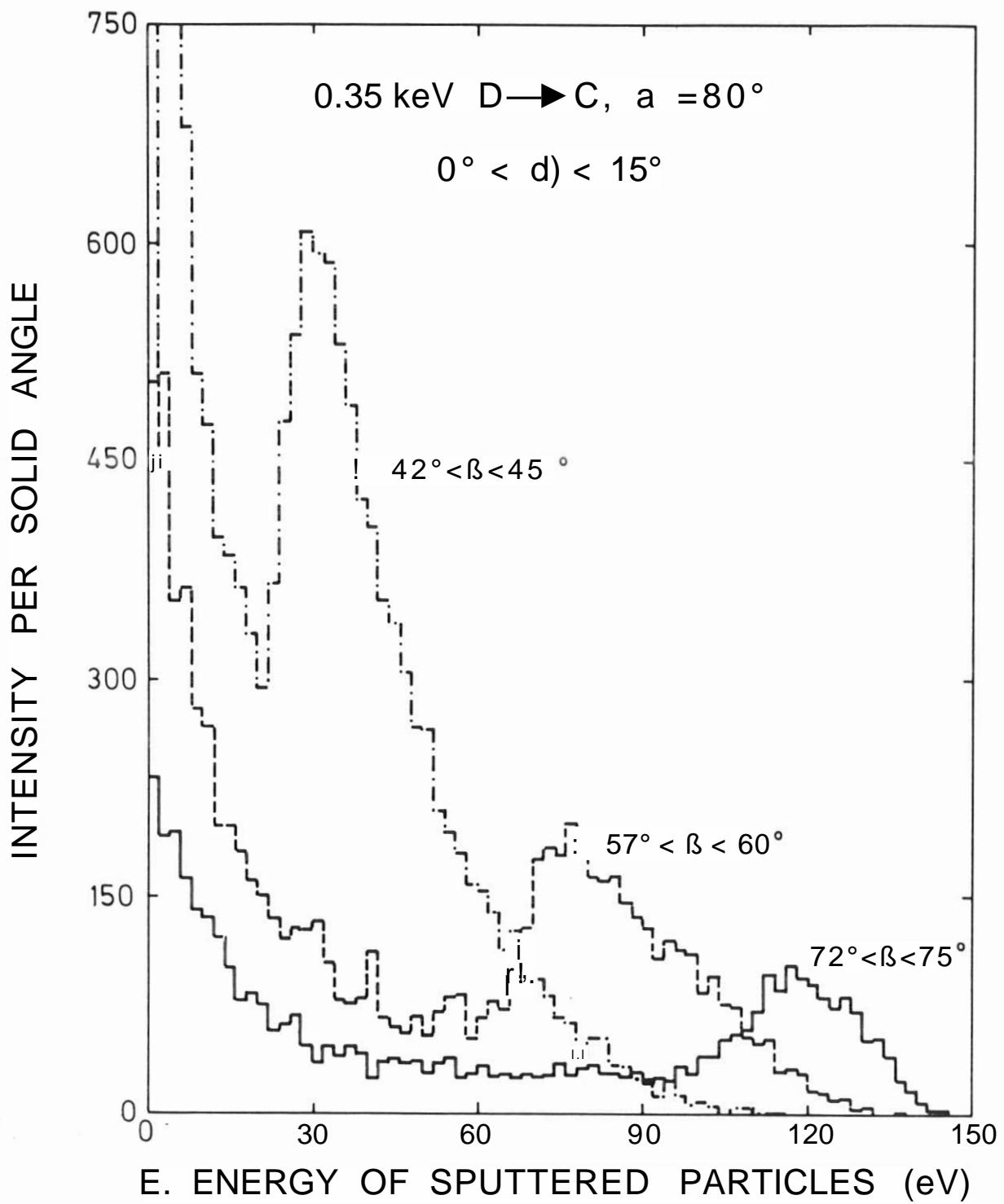


Fig. 53b

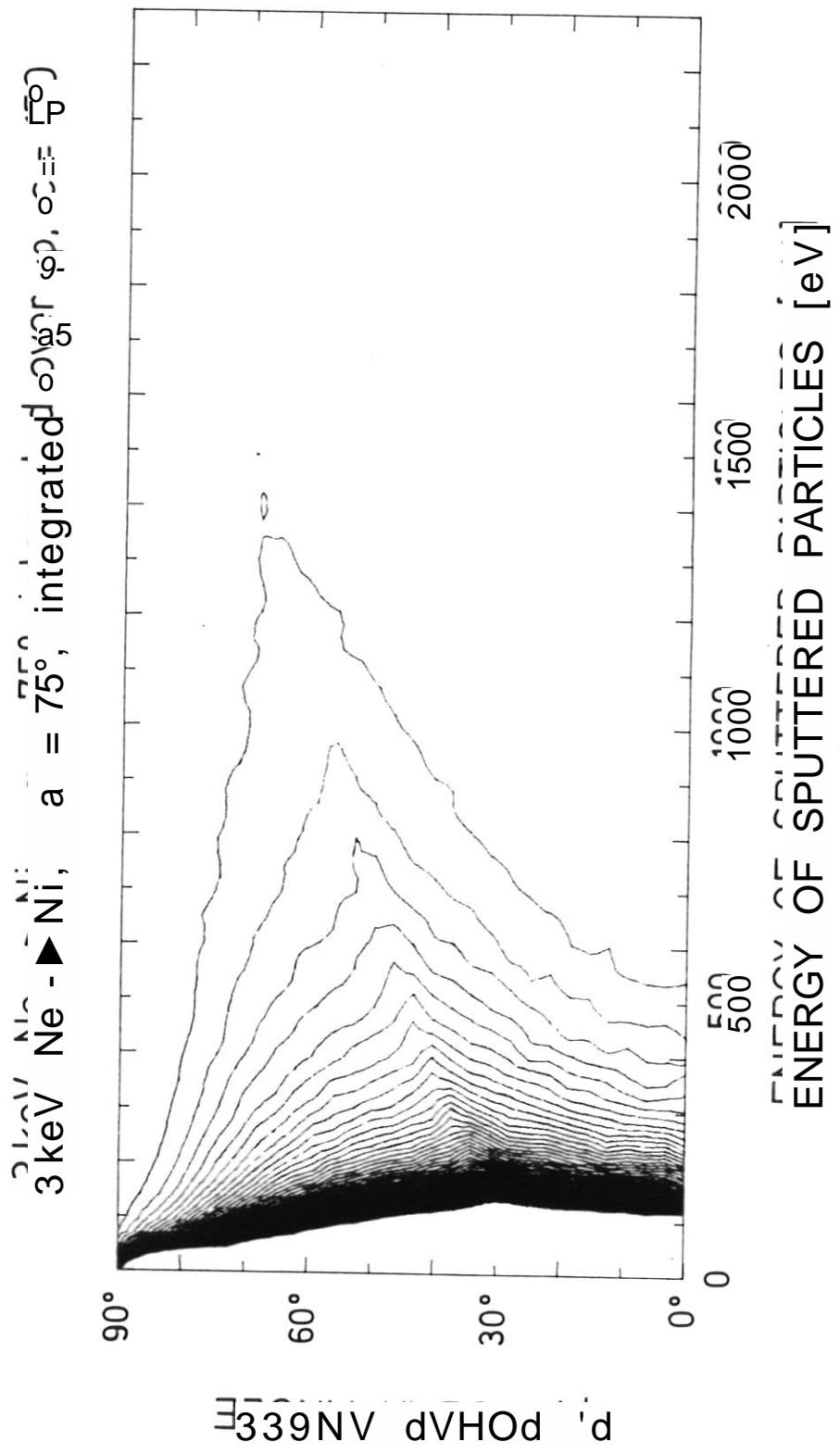


Fig. 54a

3 keV Ne  $\rightarrow$  Ni,  $\alpha = 75^\circ$ ,  $0^\circ < \theta < 15^\circ$ ,  $c = 40$

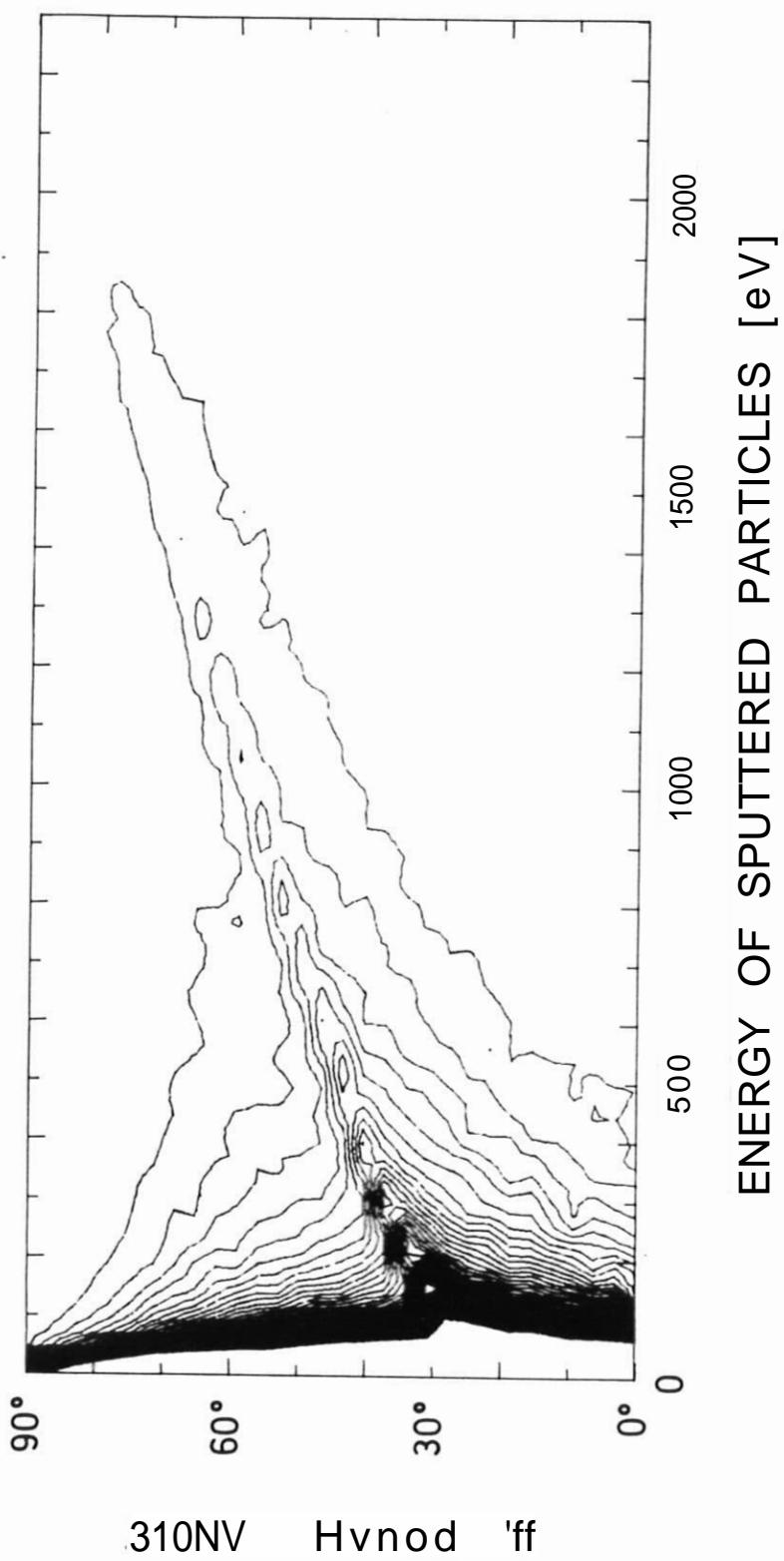


Fig. 54b

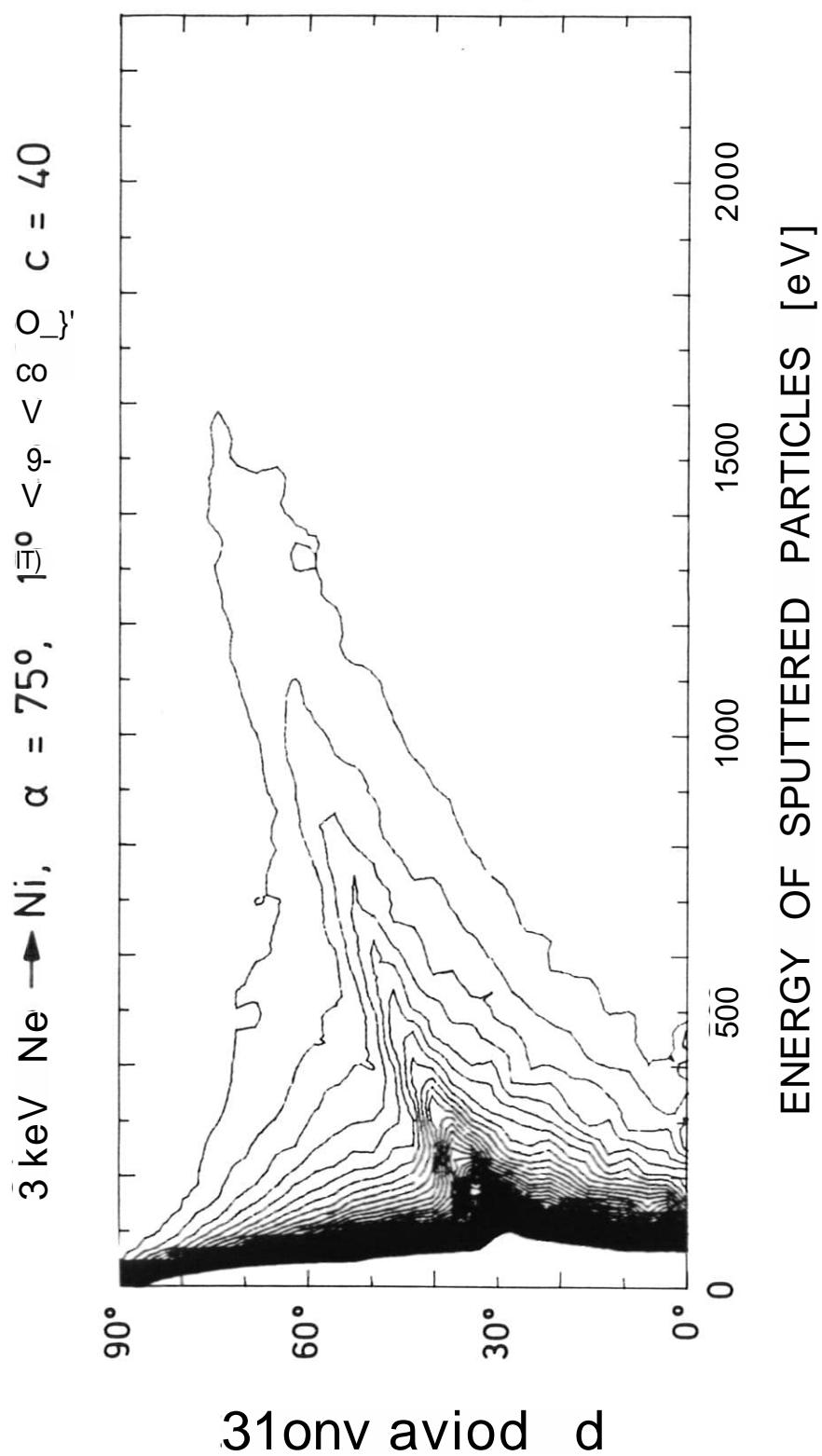
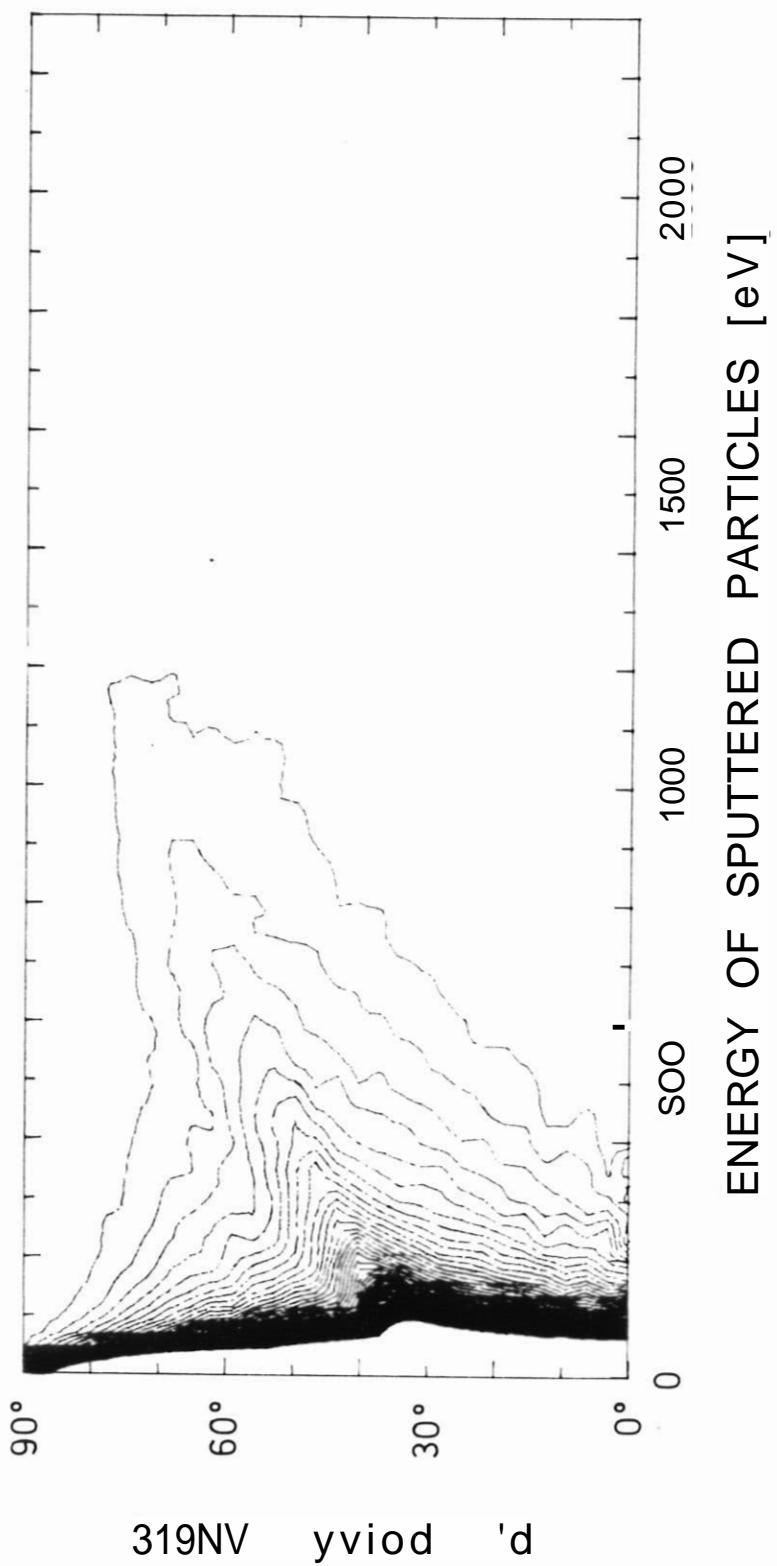


Fig. 54c

3 keV Ne  $\rightarrow$  Ni,  $\alpha = 75^\circ$ ,  $30^\circ < \vartheta < 45^\circ$ ,  $\phi = 4^\circ$



319NV yviod 'd

Fig. 54d

ENERGY OF SPUTTERED PARTICLES (eV)

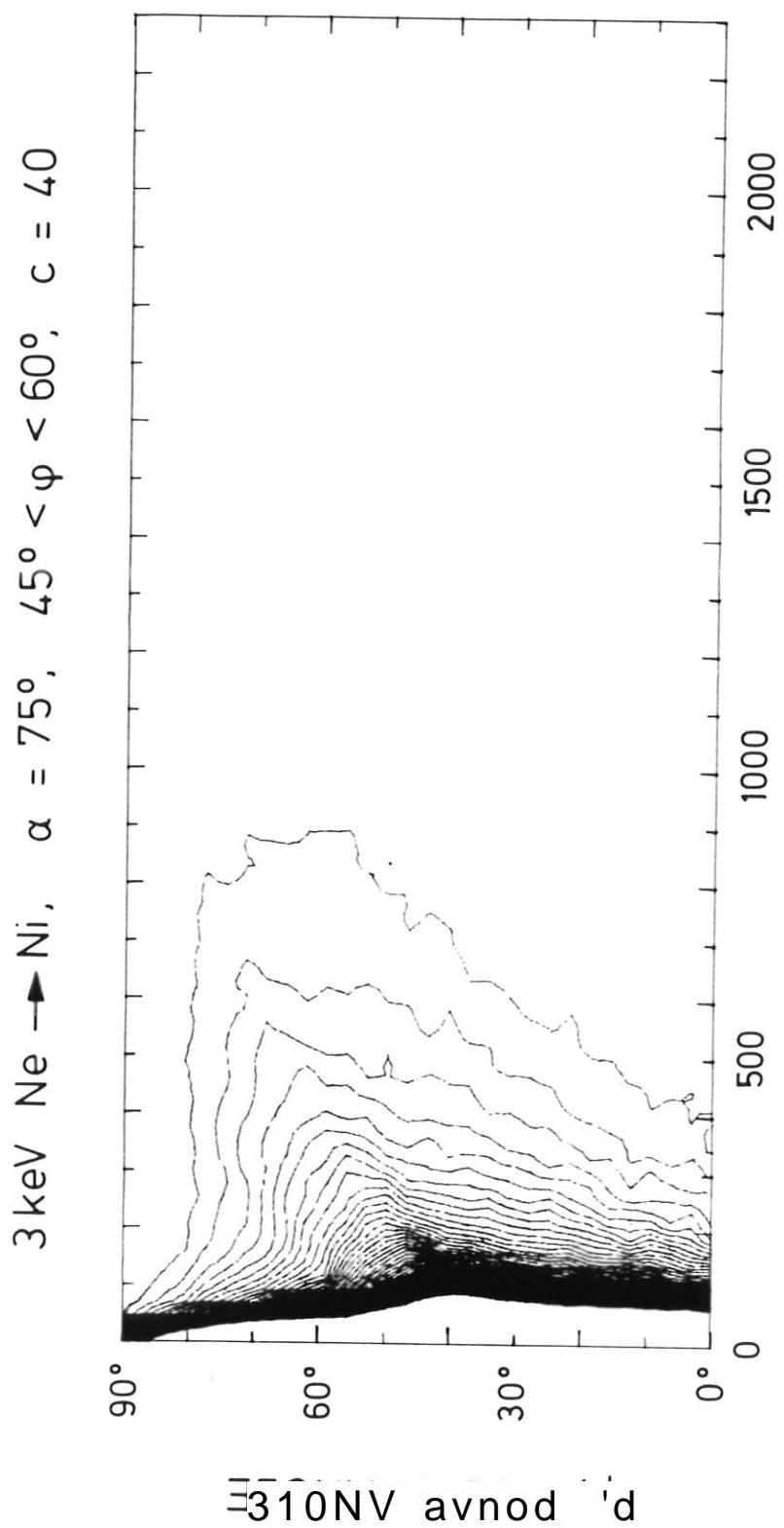
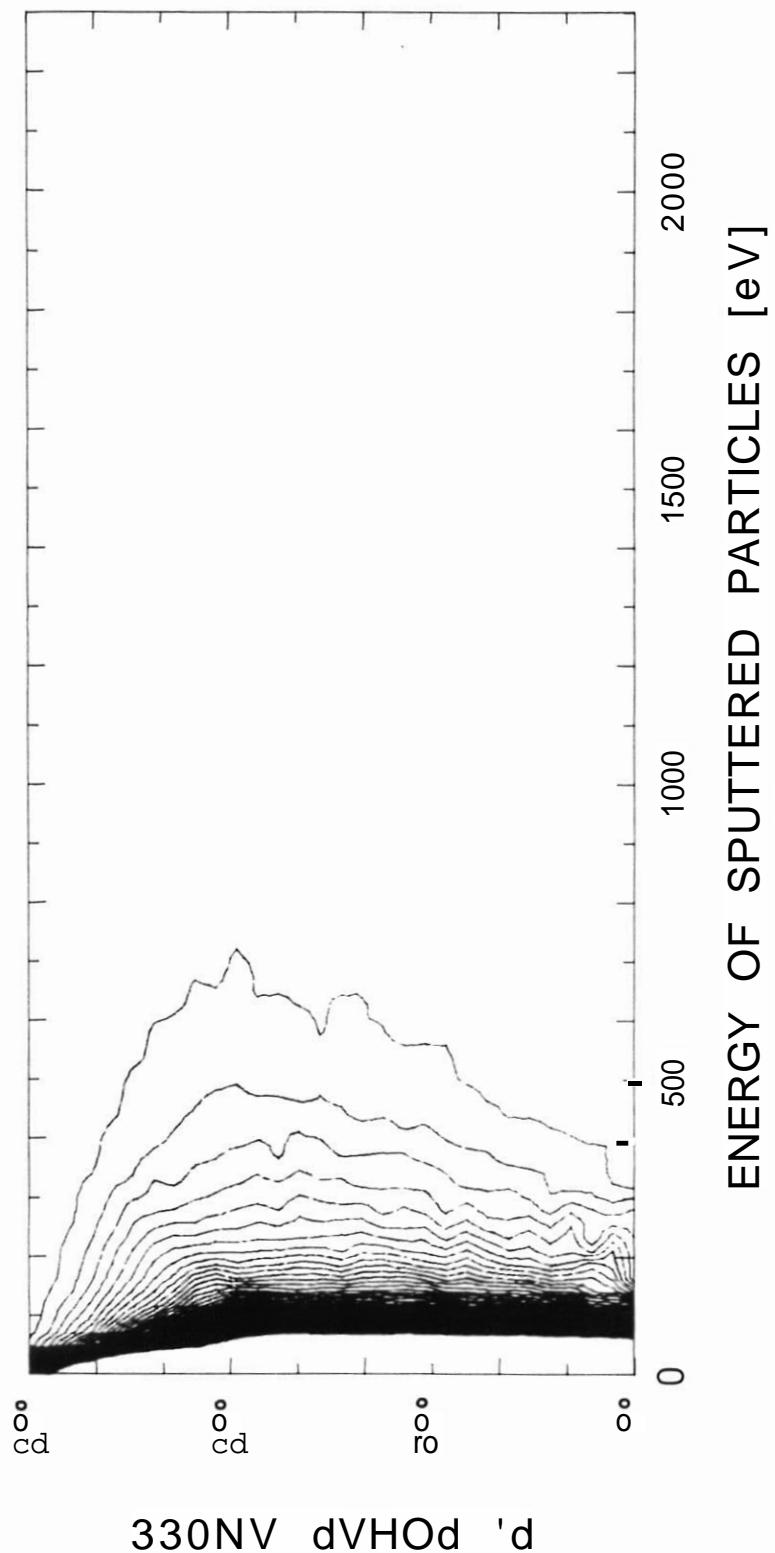


Fig. 54e

$3 \text{ keV Ne} \rightarrow \text{Ni}, \quad a = 75^\circ, \quad 60^\circ < \vartheta < 75^\circ, \quad c = 40$



330NV dVHOd 'd

Fig. 54f

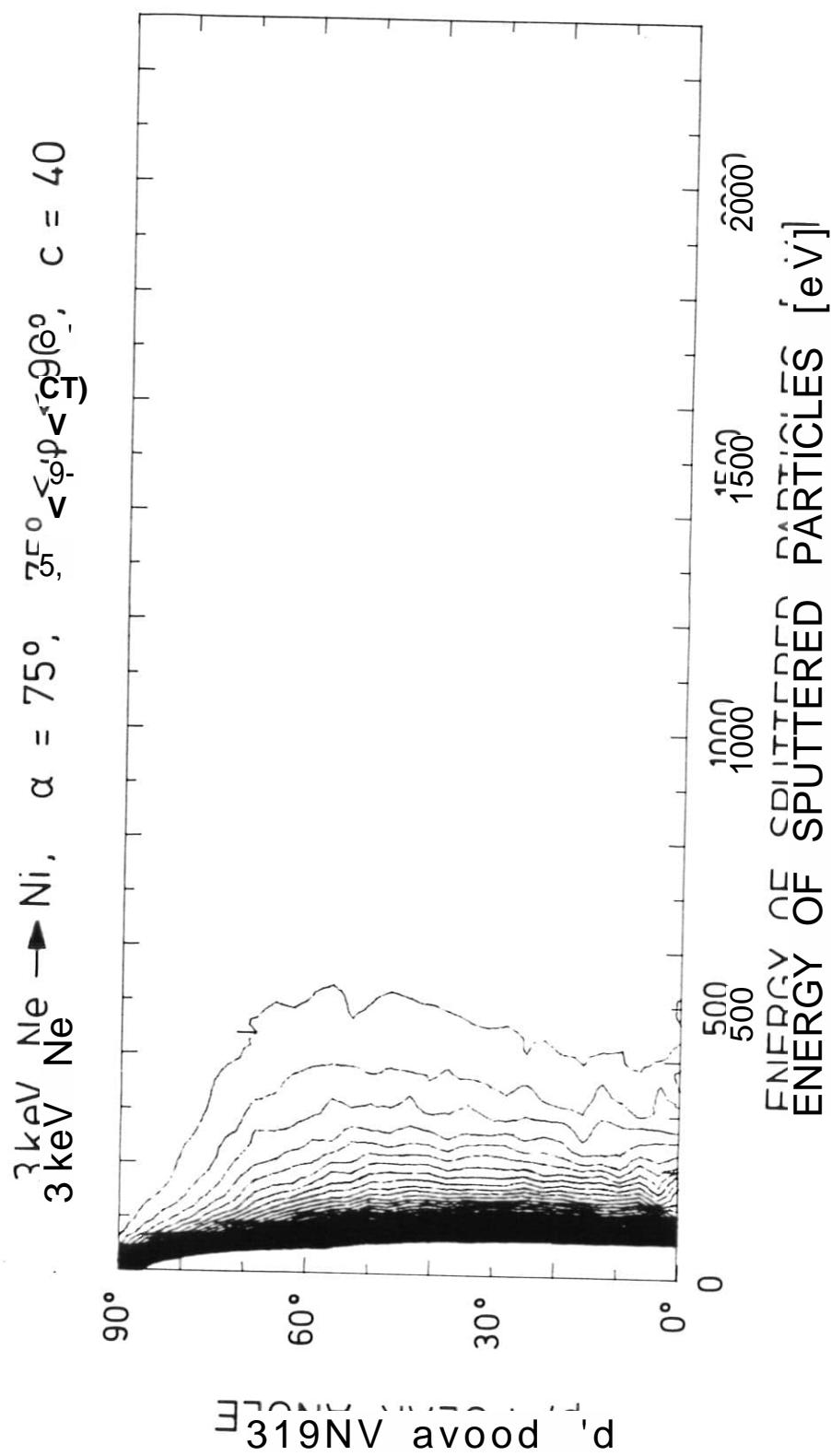


Fig. 54g

3keV Ne -►Ni.       $\alpha = 75^\circ$ ,     $90^\circ < \theta < 105^\circ$ ,    c - 40

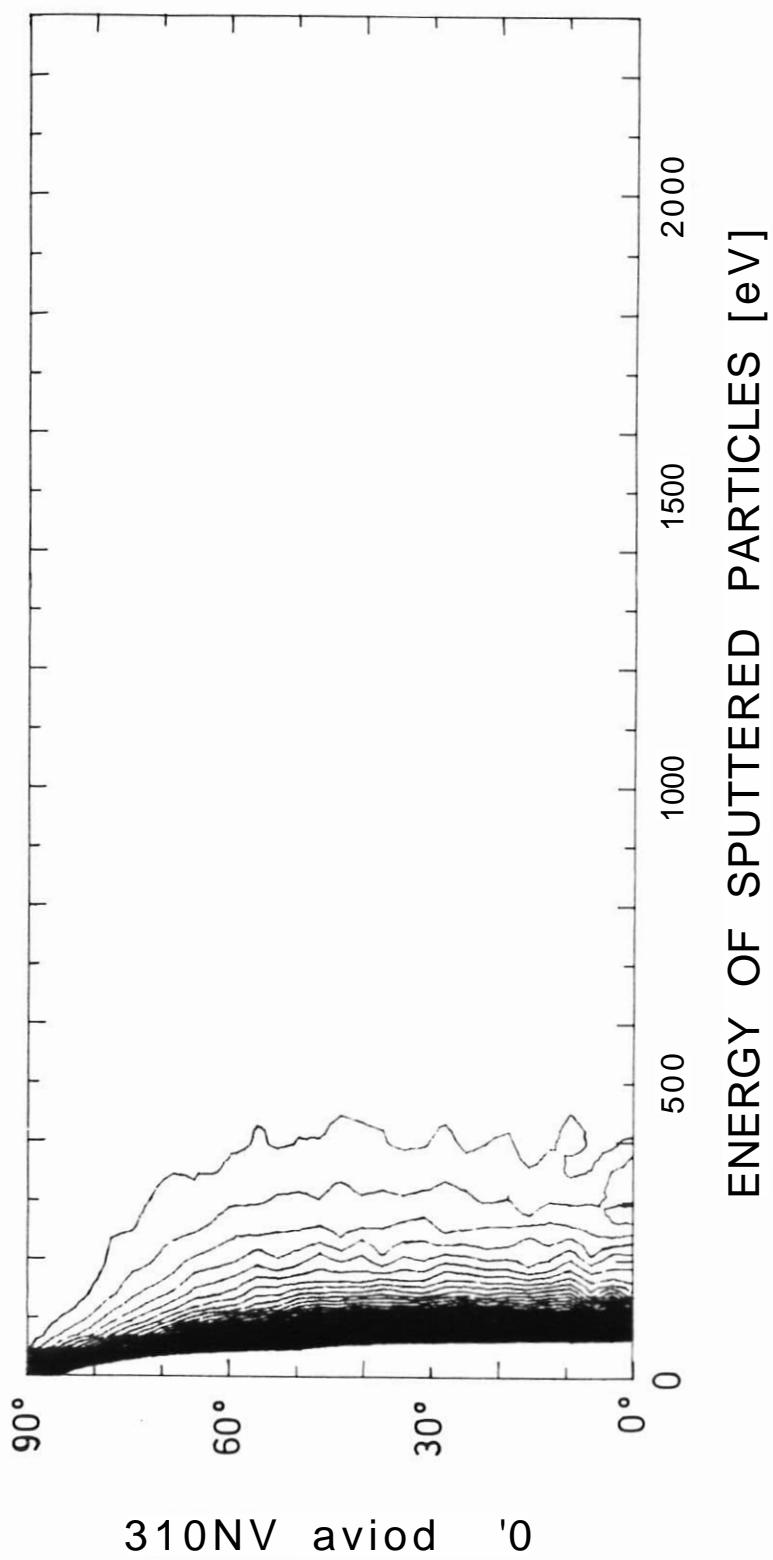


Fig. 54h

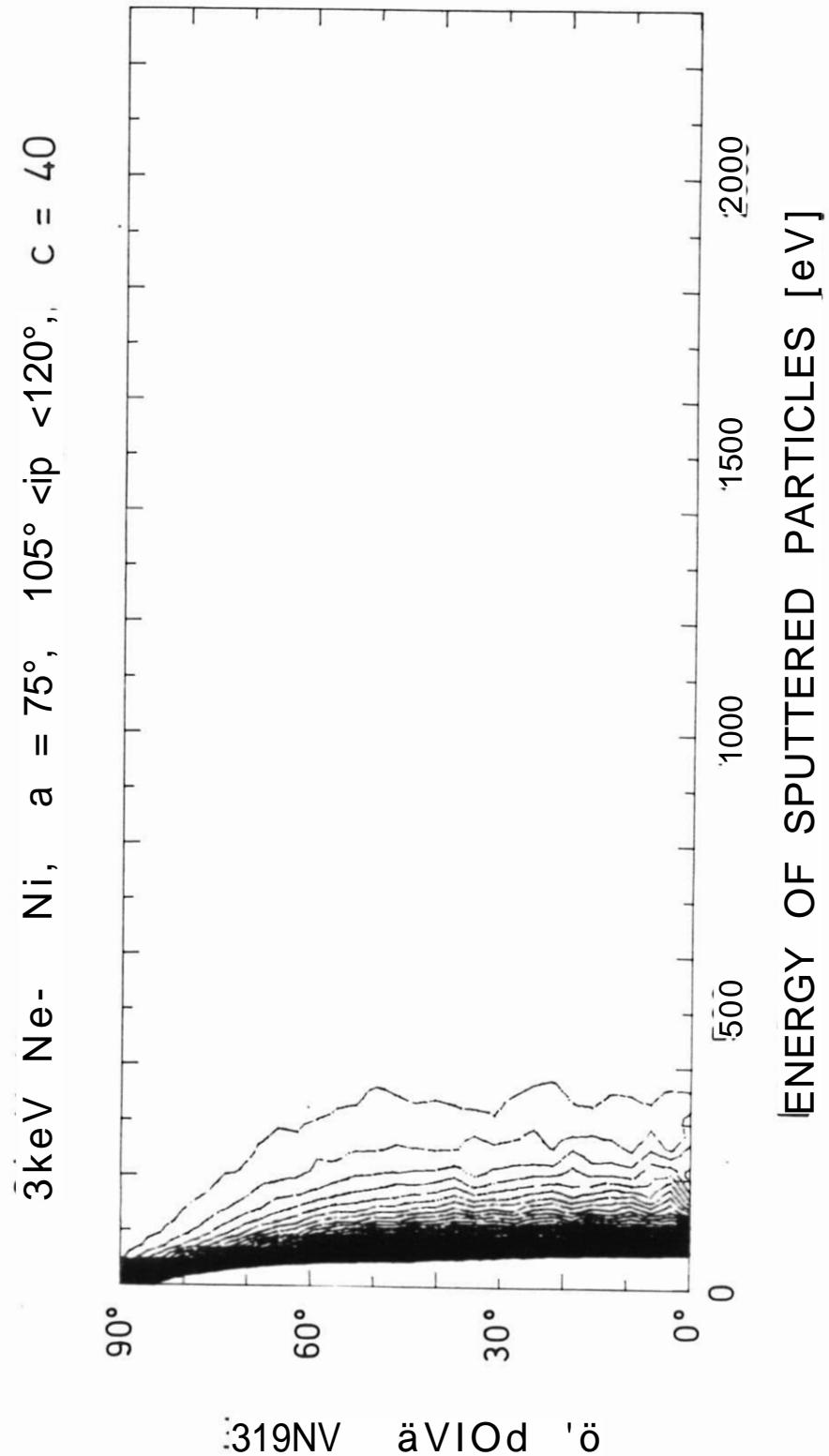


Fig. 54i

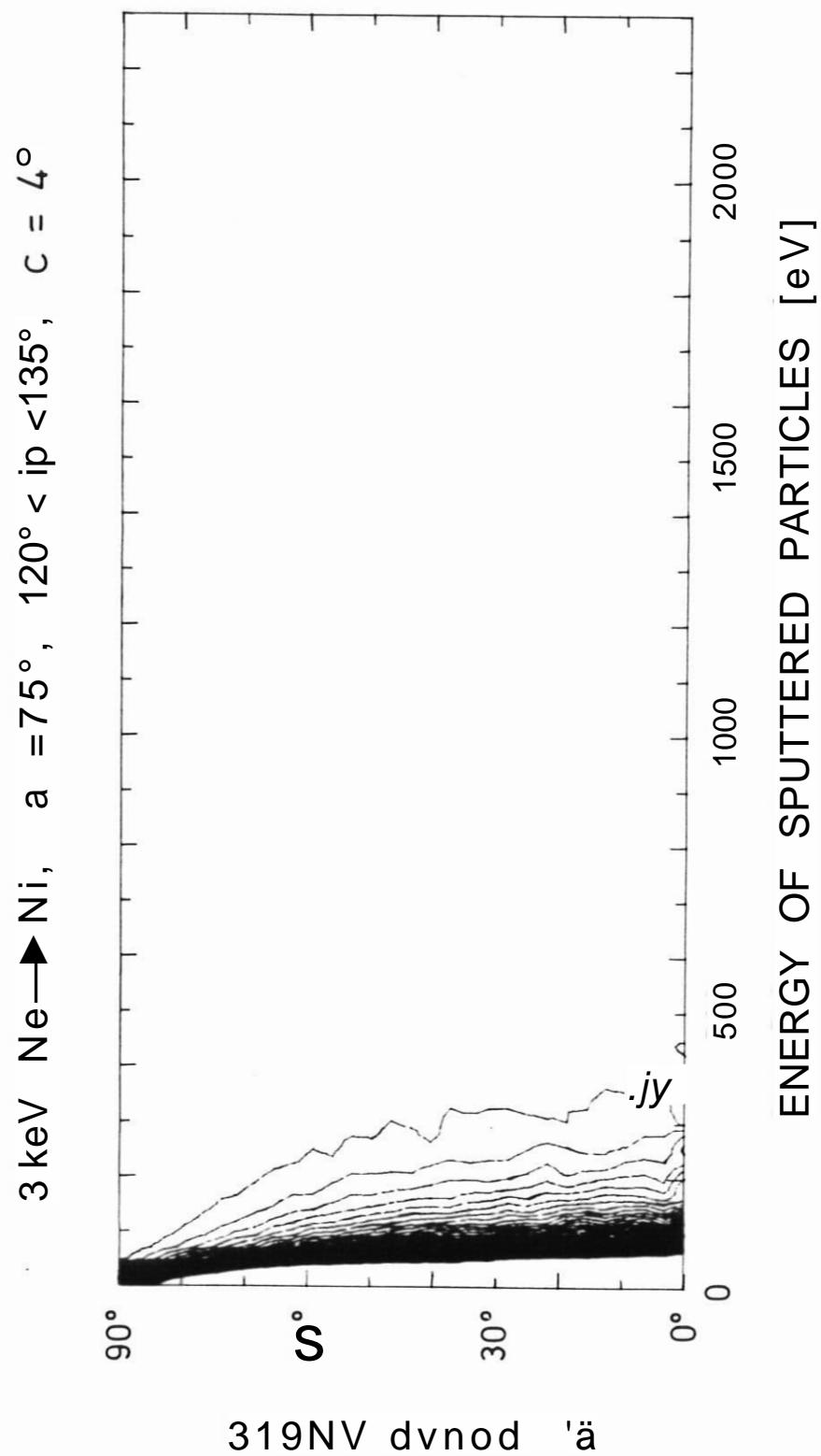


Fig. 54j

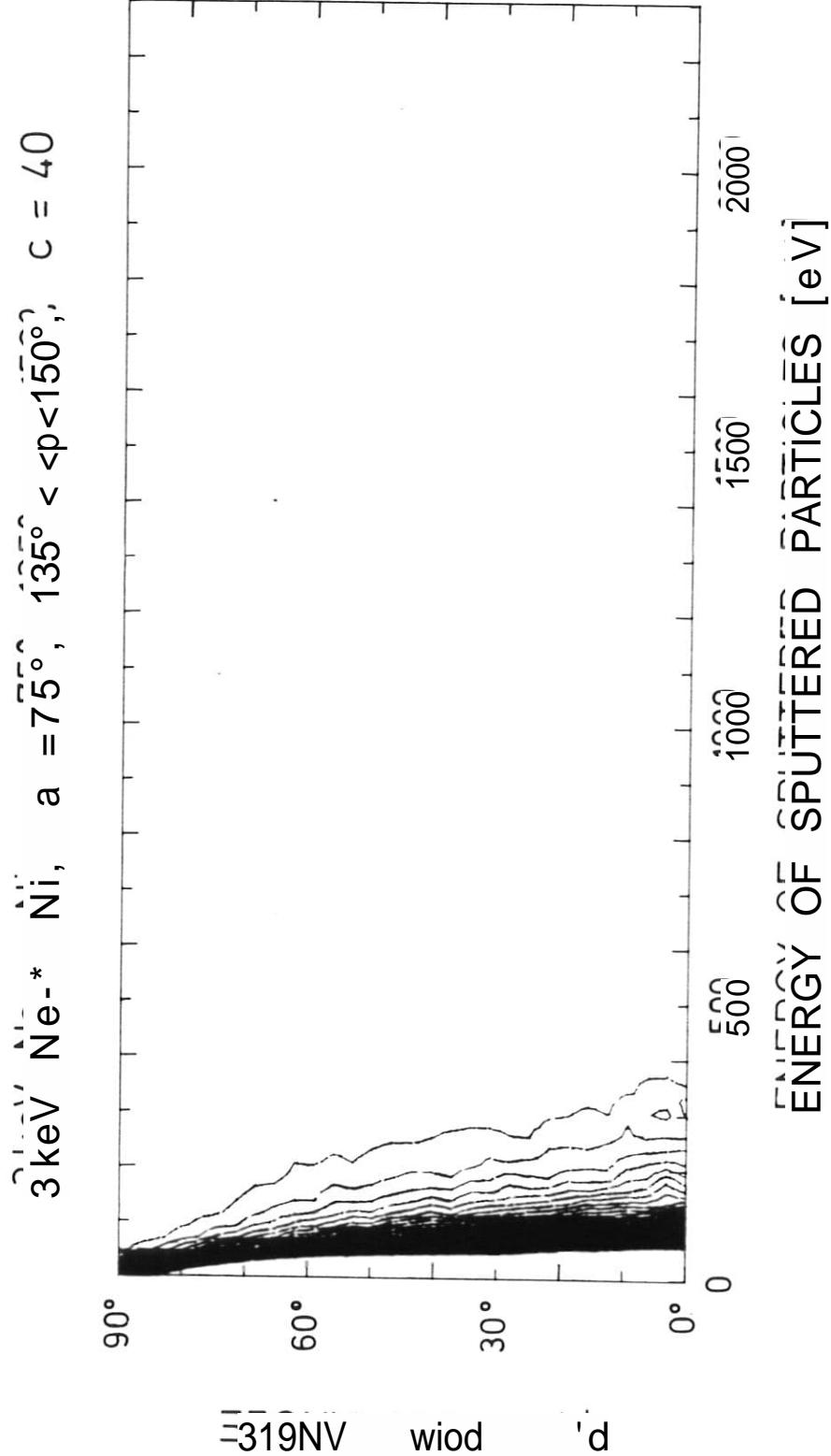
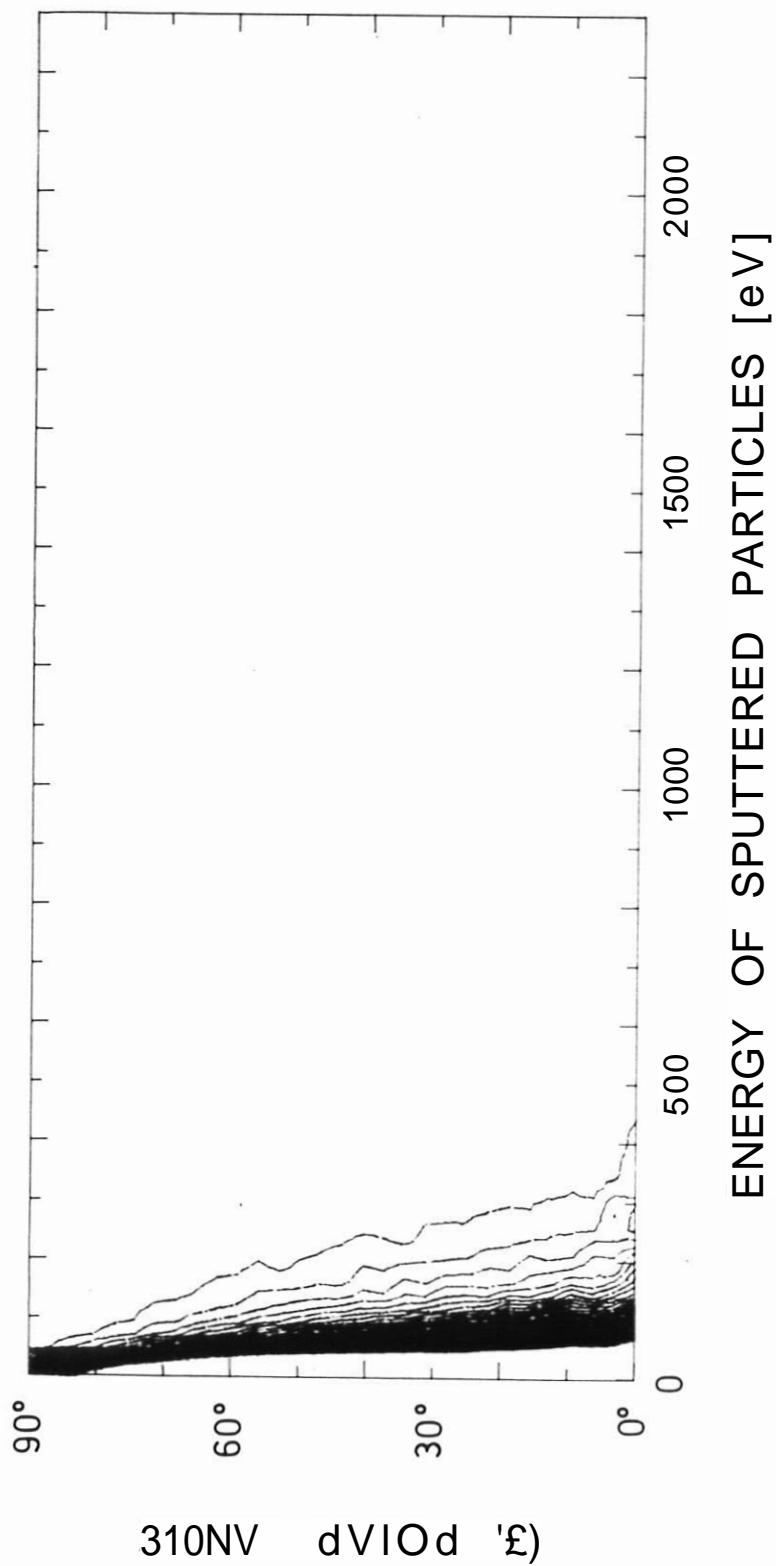


Fig. 54k

3 keV Ne  $\rightarrow$  Ni. a  $\approx$  75°.  $150^\circ < \theta < 165^\circ$ .  $\sigma = 4^\circ$



310NV dVIOd '£)

Fig. 541

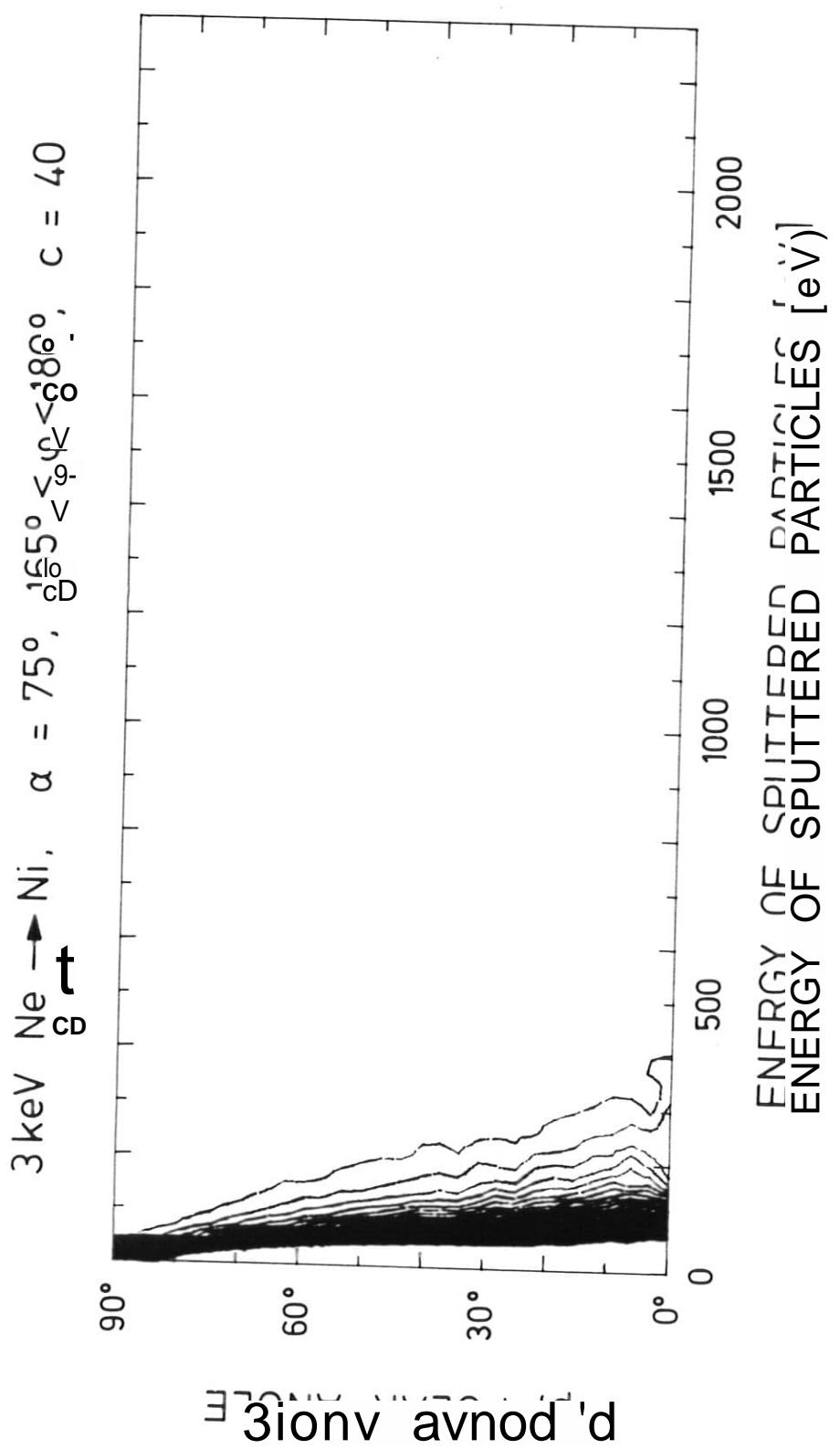


Fig. 54m

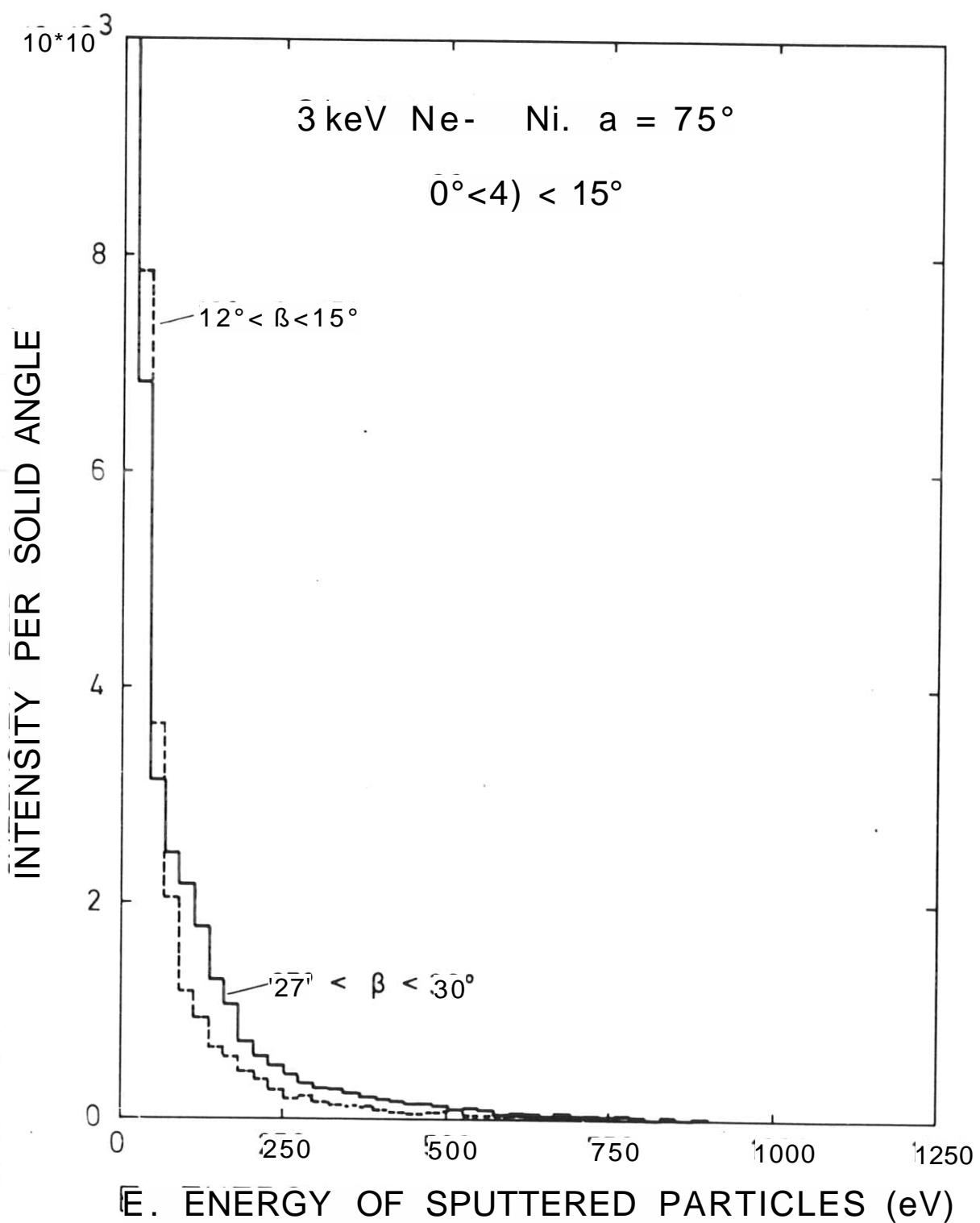


Fig. 55a

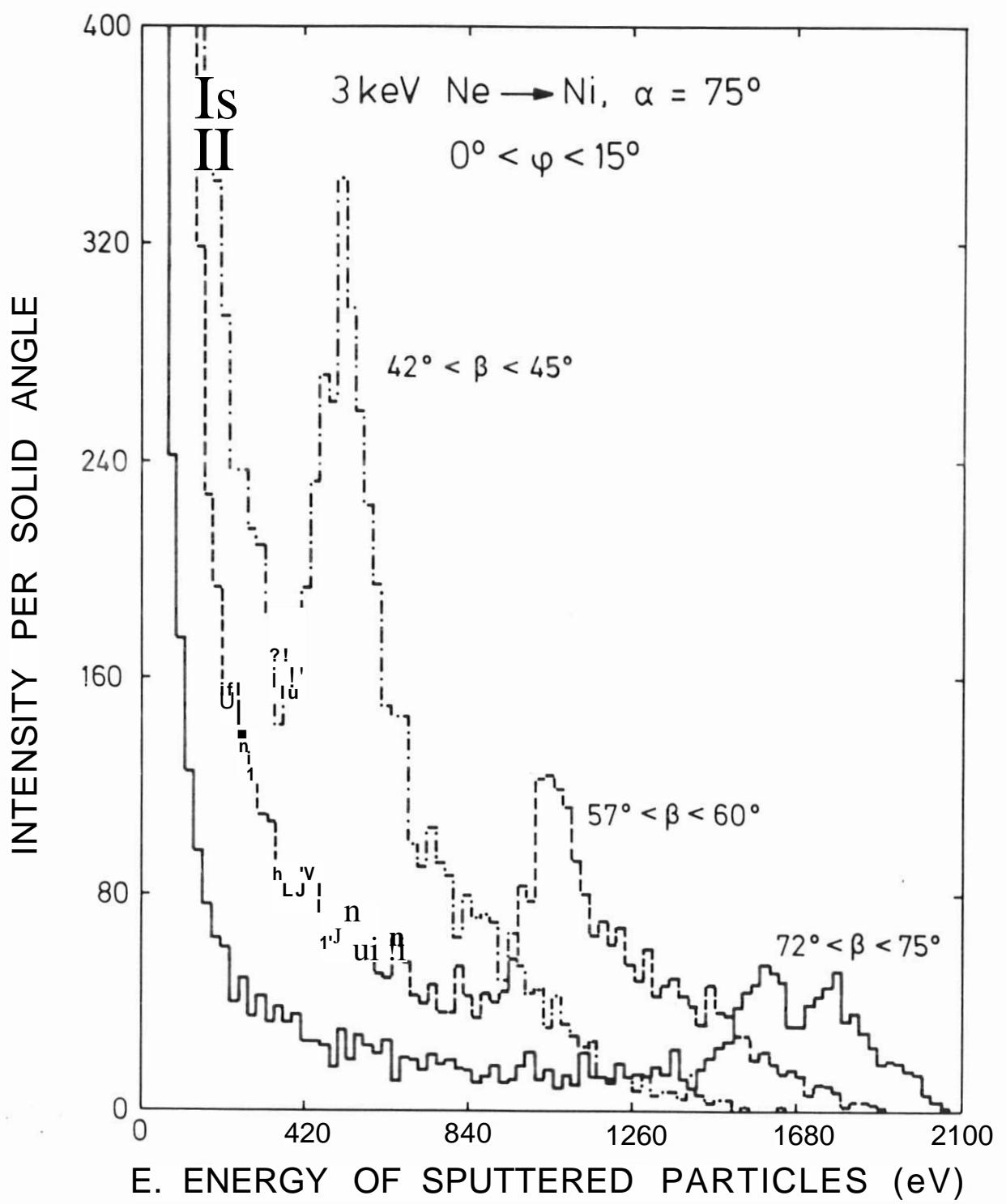


Fig. 55b

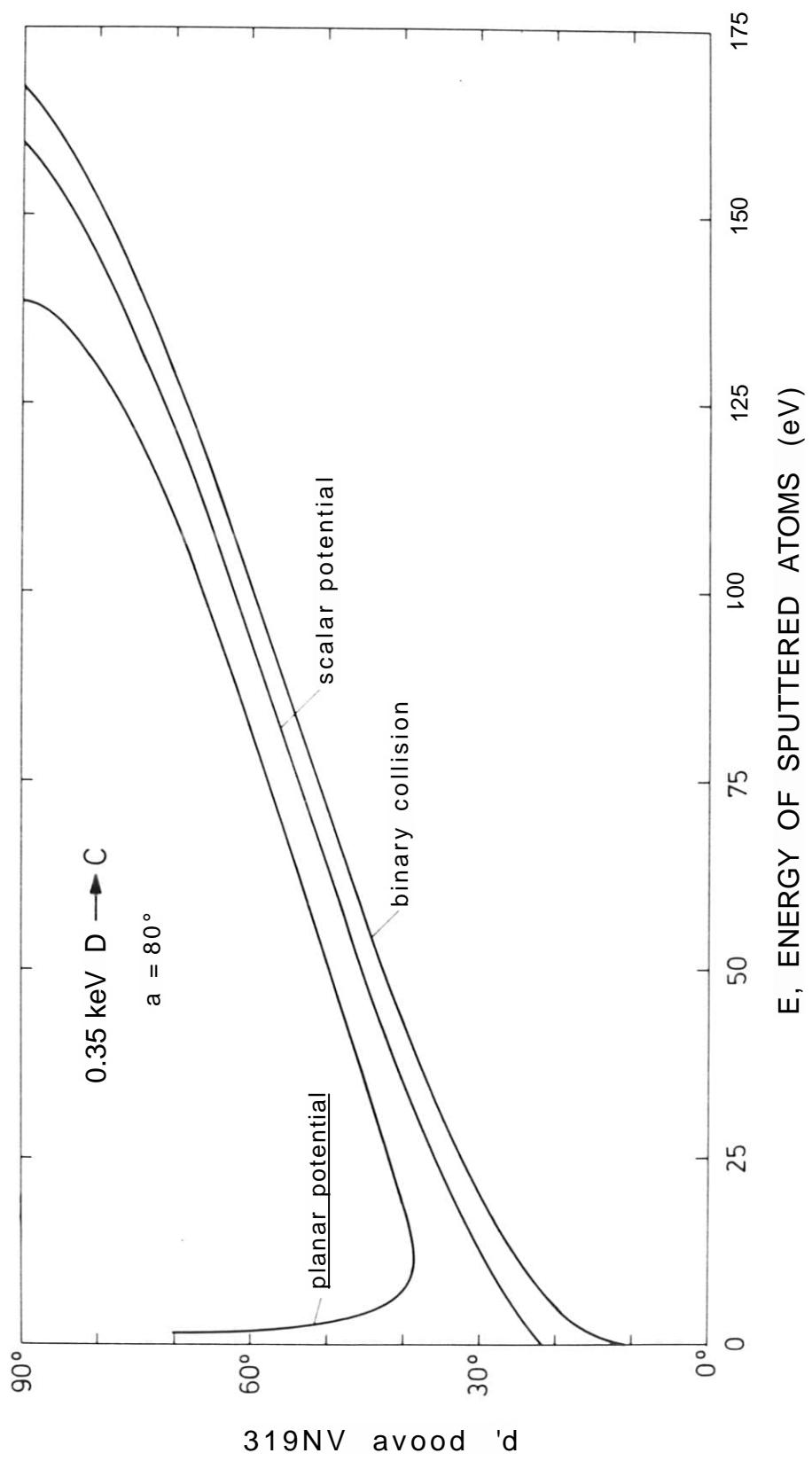


Fig. 56

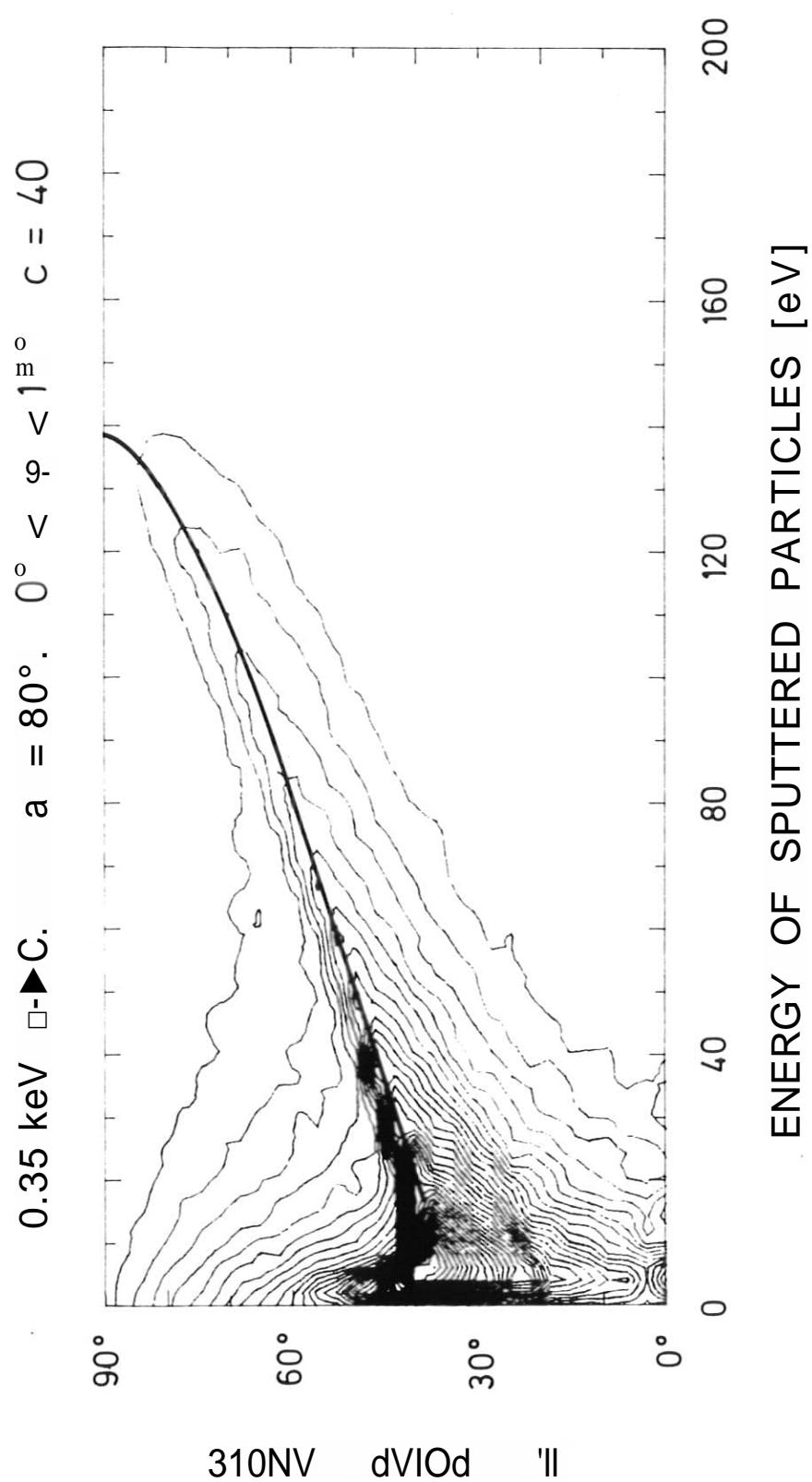


Fig. 57a

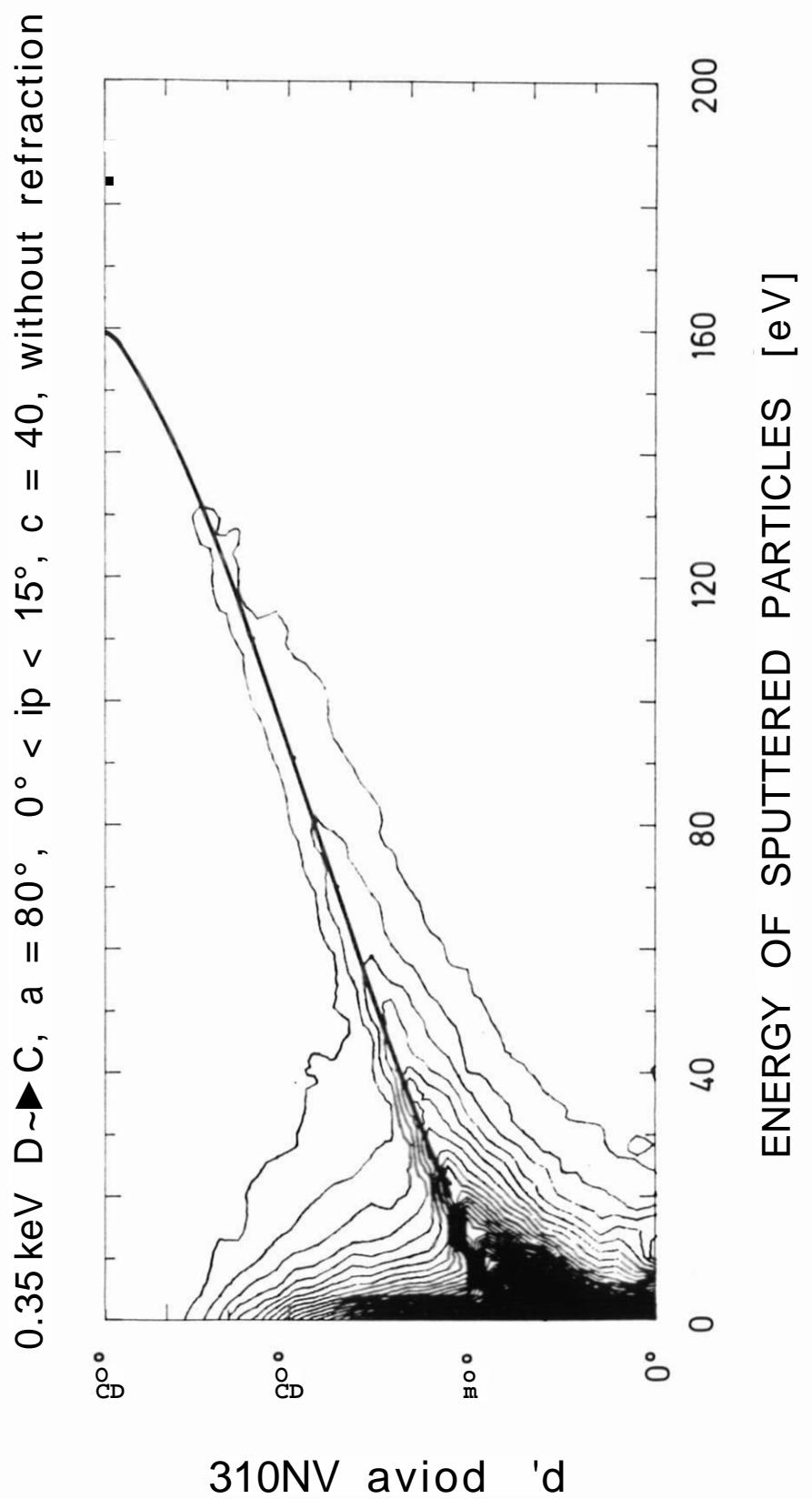


Fig. 57b

ENERGY OF SPUTTERED PARTICLES [eV]

CsI

10

15

σ

4°

0°

30°

60°

90°

339NV HVIOd '0

3 keV Ne -► Ni, θ = 75°. 0° < σ < 15°. C = 4°

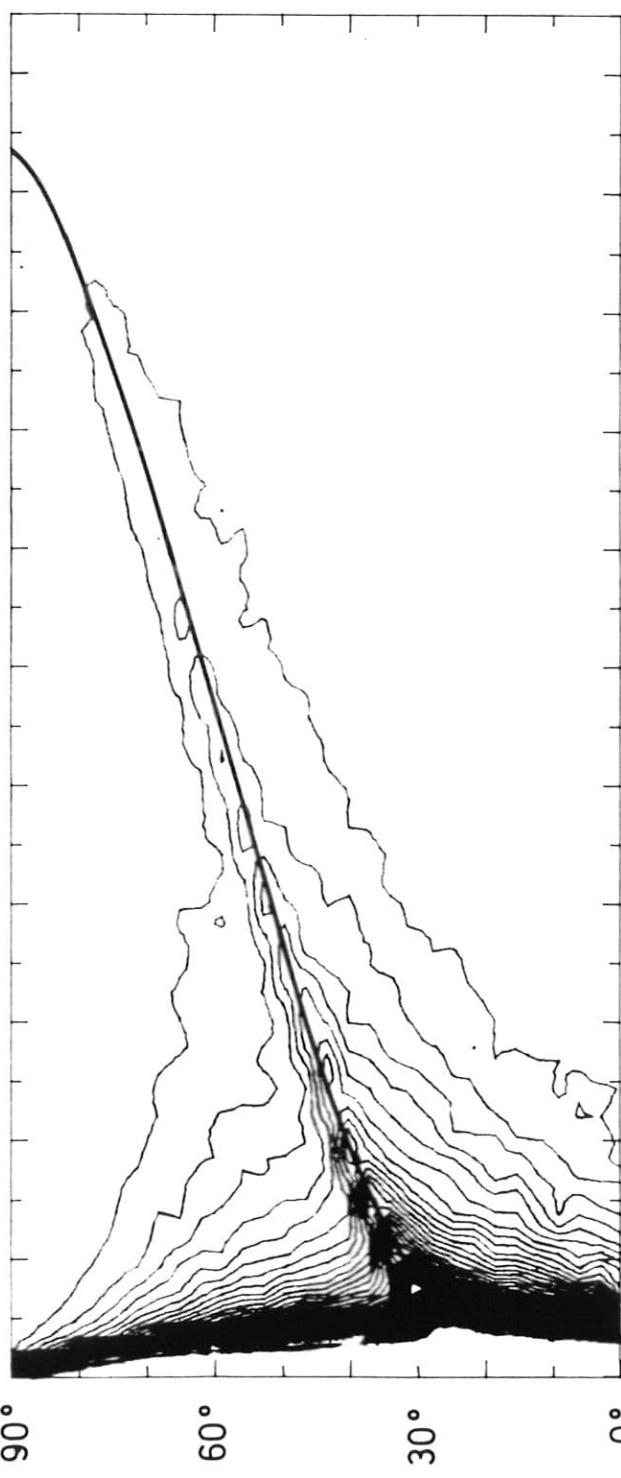


Fig. 58

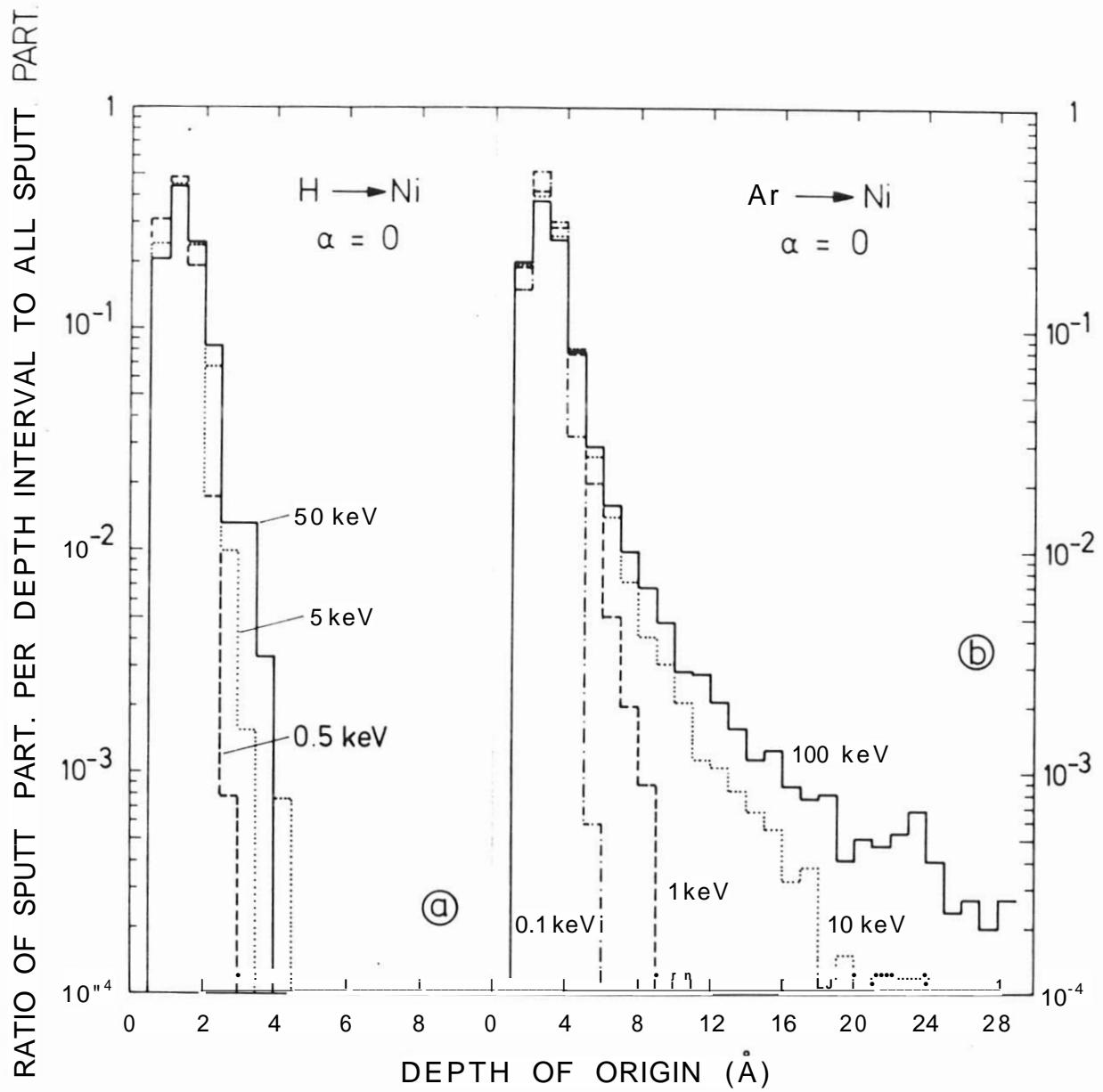


Fig. 59

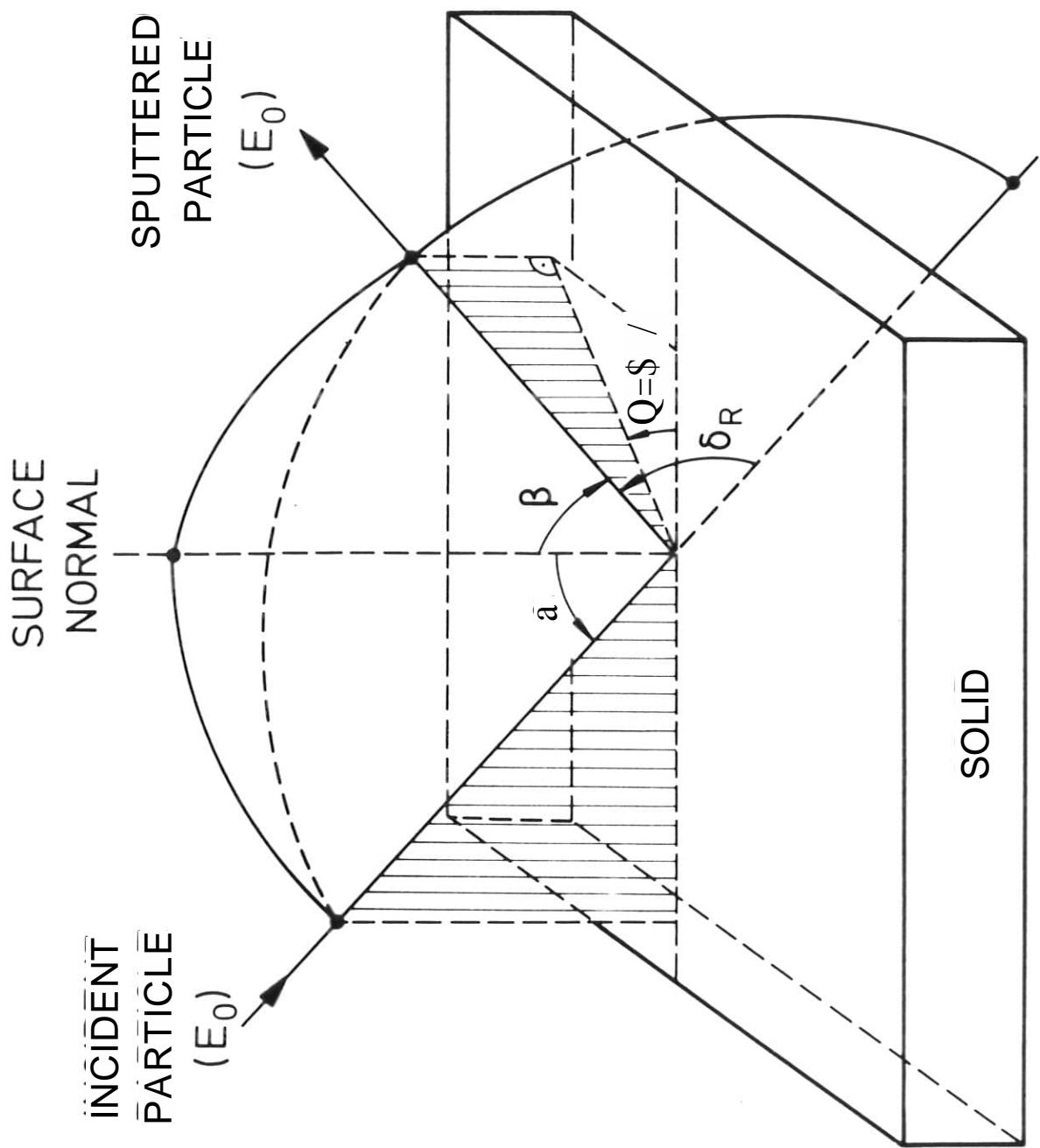


Fig. 60

initial flight  
direction

