ON PENETRATION DEPTHS AND COLLISION CASCADES IN SOLID MATERIALS

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PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR IN DE WISKUNDE EN NATUURWETENSCHAPPEN AAN DE RIJKSUNIVERSITEIT TE LEIDEN OP GEZAG VAN DE RECTOR MAGNIFICUS DR P. MUNTENDAM, HOOGLERAAR IN DE FACULTEIT DER GENEESKUNDE, TEN OVERSTAAN VAN EEN COMMISSIE UIT DE SENAAT TE VERDEDIGEN OP WOENSDAG 14 FEBRUARI 1968 TE KLOKKE 15.15 UUR

door

JACOB BAREND SANDERS

geboren te Rotterdam in 1930

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PROMOTOR:
Prof. Dr P. MAZUR

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ERRATA

On:

p. 17 in line 5 in eq. (2.37) read $p(\vec{r} - \Delta\vec{r}, \vec{n}, E)$ instead of $p(\vec{r} - \vec{r}, \vec{n}, E)$

p. 23 in eq. (3.4) read $\prod_{i=1}^{\mu} \delta(T-E_{\alpha_i})$ instead of $\prod_{i=1}^{\mu} \delta(T - E_{\alpha_1})$

and: $\prod_{i=1}^{\mu} \delta(E - T - E_{\alpha_i})$ instead of $\prod_{i=1}^{\mu} \delta(E - T - E_{\alpha_1})$

p. 25 in eq. (3.12) read $\frac{(1 - \frac{1}{s})E}{E_f^{1-\frac{1}{s}} E_1^{1+\frac{1}{s}}}$ instead of $\frac{(1 - \frac{1}{s})E}{E_f^{1-\frac{1}{s}} E^{1+\frac{1}{s}}}$

p. 26 in line 15 read (3.12) instead of (3.6)

p. 27 in line 17 read (3.12) instead of (3.14)

p. 30 in line 16 read (3.21) and (3.19) for resp. (3.27) and (4.25)

p. 30 in eq. (3.22) read $\delta(T-E_{\alpha_i})\,\delta(\zeta''_{\alpha_i}-1)$ instead of $\delta(T - E_{\alpha_1})\,\delta(\zeta''_{\alpha_1} - 1)$

and $\delta(E-T-E_{\alpha_i})\delta(\zeta'_{\alpha_i}-1)$ instead of $\delta(E-T-E_{\alpha_1})\delta(\zeta''_{\alpha_1}-1)$

p. 33 in eq. (3.36) read $\frac{1}{2}\,\frac{(1 - \frac{1}{s})}{E_f^{1-\frac{1}{s}} E_1^{\frac{1}{2}+\frac{1}{s}}}$ instead of $\frac{1}{2}\cdot\frac{(1 - \frac{1}{s})}{E_f^{1-\frac{1}{s}} E_2^{1+\frac{1}{s}}}$

p. 35 in eq. (3.45) read $\sum_{i=1}^{\nu} \sqrt{2\,m\,E_i}\,\zeta_i$ instead of $\sum_{i=1}^{\nu} \sqrt{2m\,E_1}\,\zeta_1$

p. 37 in eq. (4.4) read $\prod_{i=1}^{\mu}$ instead of $\prod_{i=1}$

p. 37 in line 14 read $W_\lambda^{(\nu)}$ instead of $W^{(\nu)}$

in line 17 read $\overline{W}(E, \vec{n}; E_1, \vec{r}_1)$ instead of $W(E, \vec{n}!/E_1, \vec{r}_1)$

in eq. (4.6) second member read $\overline{\nu}(E; E_1)$ instead of $\overline{\nu}(E, E)$

in line 19 read $\overline{\nu}(E; E_1)$ instead of $\nu(E, E_1)$

in line 20 read $\overline{W}(E, \vec{n}; E_1, \vec{r}_1)$ instead of $W(E, \vec{n}; E, \vec{r})$

p. 40 in eq. (4.12) read 0 instead of δ

p. 41 in eq. (4.14) read 0 instead of δ

p. 44 in eq. (4.28) read $B(1 - \frac{1}{s}; \frac{4}{s} + 1)$ instead of $B(r\,\frac{1}{s}\,; \frac{4}{s} + 1)$

p. 56 in third line under table (5.5) read 1000 eV instead of 100 eV.

Aan de Nagedachtenis van mijn Vader en Moeder
Aan mijn Vrouw

VOORWOORD

Teneinde te voldoen aan de wens van de Faculteit der Wiskunde en Natuurwetenschappen, volgt hier een kort overzicht van mijn studie.

In 1950 behaalde ik het einddiploma gymnasium β aan het Maerlant Lyceum te 's-Gravenhage, en begon daarna mijn studie aan de Rijksuniversiteit te Leiden. In 1954 deed ik candidaatsexamen in de wis- en natuurkunde (B), en in 1958 legde ik met goed gevolg het doctoraalexamen af, met natuurkunde als hoofdvak en wiskunde en mechanica als bijvakken.

Hierna heb ik tot 1960 gewerkt in het Weizmann Institute of Science te Rehovoth, Israël, waar ik kernspectroscopisch onderzoek heb verricht onder leiding van professor dr I. Talmi.

Nadat ik in 1960 in Nederland was teruggekeerd, ben ik in dienst getreden van het FOM-Instituut voor Atoom- en Molecuulfysica, onder directie van professor dr J. Kistemaker. Ik nam er deel aan het werk in de groep welke onderzoek verricht op het gebied van bombardement van vaste stof met snelle ionen. Mijn proefschrift bevat resultaten van het onderzoek dat ik aldaar heb verricht. Voor het bereiken van deze resultaten is de samenwerking en de discussie met vakgenoten van zeer groot belang geweest.

Ik wil hierbij in de eerste plaats noemen: mijn promotor, professor dr P. Mazur, wiens vele kritische opmerkingen op de uiteindelijke vorm van het proefschrift een grote invloed hebben gehad. De voortdurende belangstelling van, en de gedachtenwisseling met professor dr J. Kistemaker hebben een grote stimulerende werking uitgeoefend.

Van de vroegere en de huidige medewerkers aan het FOM-Instituut voor Atoom- en Molecuulfysica wil ik dr P.K. Rol, dr J.M. Fluit en dr C. Snoek noemen, met wie een zeer prettige samenwerking heeft bestaan. Speciale vermelding verdienen de vele gesprekken met drs D. Onderdelinden.

Van zeer grote betekenis voor de totstandkoming van dit proefschrift is ook geweest een verblijf van 3 maanden aan het Instituut voor Theoretische Natuurkunde te Aarhus, Denemarken, onder directie van professor dr J. Lindhard, met wie ik vele inspirerende discussies heb gevoerd.
Van de buitenlandse collega's, die door gedachtenwisseling aan dit proefschrift hebben bijgedragen, wil ik gaarne noemen: professor dr M.W. Thompson, dr P. Sigmund en dr S. Datz.

Ik wil, tot slot, niet nalaten om mejuffrouw M.J. Benavente te bedanken voor het vervaardigen van de tekeningen, de heer F.L. Monterie voor het fotografische werk, mejuffrouw J.M. de Vletter en mevrouw C.J.Köke-van der Veer voor het typen van het manuscript, en mejuffrouw A. Klapmuts voor de veelvuldige hulp bij administratieve problemen.

CONTENTS

CHAPTER I

INTRODUCTION

The field of radiation damage and sputtering has been studied by many authors [1,2]. Radiation damage and sputtering are the phenomena which occur when a solid target is bombarded with ions which have been accelerated to a high kinetic energy. This kinetic energy will be supposed to have a value between 20 and 50 keV in all cases which will be discussed in this thesis.

When such a projectile enters the target, it will collide with other atoms, to which it will transfer kinetic energy. These, in their turn, will collide with other atoms and so on. In this way a collision cascade originates in the target. If the target has a crystalline structure, this cascade causes destruction in the lattice, which is called radiation damage. Also some atoms can be ejected from the target in the course of the cascade and this is called sputtering. For short historical surveys of this phenomenon we refer to the theses of Rol [3], Fluit [4] and Weysenfeld [5].

In this thesis we shall study the ranges (i.e. the distances travelled) of energetic projectiles and the collision cascades caused by them. We have not the intention of making explicit radiation damage calculations (e.g. the average number of Frenkel pairs created by an incoming projectile), but to discuss the distribution of energies and momenta of the recoil atoms in the cascade, from which such results may be derived. Previous calculations on collision cascades have been made by Leibfried [6] and Robinson [7,8]. Leibfried has considered the recoil energy distribution function in a single crystal with a hard sphere model for the interatomic interaction, while Robinson has used other potentials for this interaction, but has limited his calculations to amorphous material.

Previous calculations of moments of ranges have been made by Leibfried [9] and Mika [10], who used a hard sphere model, by Lindhard and co-workers [11], who performed machine calculations on the basis of a Thomas Fermi potential for the interatomic interaction and by Baroody [12], who used both this model and the power-law interaction which will be described in this chapter. Baroody considers the case that projectiles start from an infinitely extended plane inside an amorphous medium with only one energy but in all possible directions with respect to the normal on the surface. He then calculates moments of the distance from the planar source, reached by these projectiles, up to the fourth order averaged over the cosine of the angle with the normal made by their initial direction of motion.

If a projectile, which in most cases is a noble gas ion, enters a single crystalline target in a transparent direction, it has a considerable probability of penetrating into a very great depth through the open space between the rows of atoms in the crystal [13,14]. This is called channeling and will not be treated here.

In this thesis we shall consider only monatomic target material, unless otherwise stated. Furthermore the calculations will be based on a model which takes into account two-body collisions only. As argued by Bohr[15] and Lindhard[11], atomic interactions in solids at relative energies in the range from 10 to 50 keV are described with a satisfactory degree of accuracy with an interatomic potential of the form

$$(1.1) \qquad V(r) \sim r^{-s}$$

r being the distance between the centers of the atoms and s lying between 2 and 4. In particular the case s = 2 is often used, because of simplifications in the necessary mathematics, which occur in this case. The potential (1.1) can be interpreted as a screened Coulomb potential.

$$(1.2) \qquad V(r) = \frac{Z_1 Z_2 e^2}{r} U(r/a)$$

with the screening function $U(r/a) = \frac{k_s}{s}\left(\frac{a}{r}\right)^{s-1}$ where k_s is a constant of the order unity.

Z_1 and Z_2 are the charge numbers of projectile and target atom respectively and a is a length which acts as an effective screening radius. Following Lindhard we shall use for a the expression:

$$(1.3) \qquad a = a_o \,.\, 0.8853\,(Z_1^{2/3} + Z_2^{2/3})^{-\frac{1}{2}}$$

where a_o is the radius of the first Bohr orbit. The constant factor k_s is of the order of 1 and may be used as a fitting parameter in a comparison with experimental results.

For this potential, Lindhard[16] has derived an approximate form for the differential cross section $d\sigma$ giving the probability that the projectile will suffer a collision in which an energy between T and T + dT is transferred to a target atom, which is

$$(1.4) \qquad d\sigma = \frac{\pi}{s}\left\{\frac{b^2}{4}\, a^{2s-2} k_s^2\, \gamma_s^2\, T_m\right\}^{1/s} \frac{dT}{T^{1+1/s}}$$

The derivation of this formula will be given in Appendix A.

In (1.4) b is Bohr's collision diameter $b = \frac{2 Z_1 Z_2 e^2}{m_o v^2}$, where m_o is the reduced mass $m_o = \frac{m_1 m_2}{m_1 + m_2}$, v is the relative velocity, T is the energy, transferred in the collision and $T_m = \frac{4 m_1 m_2}{(m_1 + m_2)^2}\, E = \gamma E$ with E the initial energy of the projectile is the greatest energy transfer possible in a single collision. m_1 and m_2 are the masses of respectively projectile and target particle. As for the remaining constant in (1.4), it is an Euler Beta function

$$\gamma_s = \tfrac{1}{2} B\left(\tfrac{1}{2}; \frac{s+1}{2}\right) \quad .$$

Often it will be necessary to introduce explicitly an angle dependent differential cross section $d\sigma'$, related to the angular and energy distribution of the participants in the collision after the scattering. From the energy - and momentum conservation - laws it can be shown that this can be done in the following way [1,9]

$$(1.5) \qquad d\sigma' = d\sigma . \delta\left(\vec{n}.\vec{n}' - \sqrt{\frac{E-T}{E}}\,\frac{m_1+m_2}{2m_1} - \sqrt{\frac{E}{E-T}}\,\frac{m_1-m_2}{2m_1}\right)$$

$$\delta\left(\vec{n}.\vec{n}'' - \frac{m_1+m_2}{2\sqrt{m_1 m_2}}\sqrt{T/E}\right)\frac{d\Omega' d\Omega''}{2\pi 2\pi}$$

In this formula $\vec{n}.\vec{n}'$ and $\vec{n}.\vec{n}''$ are the scalar products of the unit vector $\vec{n}$ in the direction of notion of the projectile before the scattering with the unit vectors $\vec{n}'$ and $\vec{n}''$ respectively in the direction of motion of the projectile and of the hit particle after the scattering. $d\Omega'$ and $d\Omega''$ are differential solid angles corresponding to the scattered directions $\vec{n}'$ and $\vec{n}''$ as given above. The factors $(2\pi)^{-1}$ are normalizations.

Integrating (1.5) over $d\Omega''$, the direction of motion of the hit particle, we obtain the quantity which characterizes the angular distribution of the projectile alone

$$(1.6a) \qquad d\sigma_1' = d\sigma\delta\left(\vec{n}.\vec{n}' - \sqrt{\frac{E-T}{E}}\,\frac{m_1+m_2}{2m_1} - \sqrt{\frac{E}{E-T}}\,\frac{m_1-m_2}{2m_1}\right)\frac{d\Omega'}{2\pi}$$

and conversely by integrating over $d\Omega'$ we get the analogous one for the angular distribution of the hit particle alone

$$(1.6b) \qquad d\sigma_2' = d\sigma\delta\left(\vec{n}.\vec{n}'' - \frac{m_1+m_2}{2\sqrt{m_1 m_2}}\sqrt{T/E}\right)\frac{d\Omega''}{2\pi} \quad .$$

For the further developments it is necessary to consider the relation between the differential cross section (1.4) and the function $K(E,T)\,dT$, which gives the probability that a particle of kinetic energy E will transfer an energy between T and $T + dT$ in a single collision. As we have excluded many-body interactions from our calculations, $K(E,T)$ is necessarily normalizable to unity

$$(1.7) \qquad \int K(E,T)\,dT = 1 \quad .$$

It is evident from (1.4) that the total cross section $\int_0^{\gamma E} d\sigma$ is infinite.

The integral diverges at the lower limit. It will turn out in the following chapters that this does not prevent us from calculating the quantities in which we shall be interested. However, for the clarity of the argument, we shall cut off the total cross section at the lower limit at some Δ, which may be taken arbitrarily small. Then the function K (E,T) is defined as

$$K(E,T)dT = \frac{d\sigma(E,T)}{\int_{\Delta}^{\gamma E} d\sigma(E,T)} \tag{1.8}$$

from which (1.7) follows at once. An explicit calculation of K (E,T) gives the result

$$K(E,T) = \frac{T^{-1-1/s}}{s(\Delta^{-1/s} - (\gamma E)^{-1/s})} \tag{1.9}$$

We must discuss the question of the applicability of classical mechanics to these collisions. This question has been treated in great detail by Niels Bohr[15], and a clear summary of it has been given by Rol[3]. Here we shall mention only the results.

The first condition is

$$b >> {}^{\lambda}/2\pi \tag{1.10}$$

which means that the De Broglie wavelength must be small compared to the effective range of the interaction for which b, which has the meaning of the distance of closest approach in a head-on collision with Coulomb-interaction, is a measure.

The second condition is

$$\theta >> \frac{\lambda}{2\pi a} \tag{1.11}$$

where θ is the scattering angle in the center of mass system. For scattering angles of the order $\lambda/2\pi a$, the uncertainty in the angle, due to the Heisenberg principle becomes of the same order as the angle itself. We give a few values of the parameters $k = b/\lambdabar$ and $\xi/k = \lambdabar/a$ (ξ is the symbol, generally used for the ratio b/a).

Table

Species	E	k	$\lambdabar/a$	T_{min}
Kr on Al	160 keV	3412.7	0.0002	$1.6 \cdot 10^{-3}$ eV
Kr on Al	40 keV	6825.4	0.0004	$1.6 \cdot 10^{-3}$ eV
Ar on Cu	50 keV	4651.5	0.0006	$4.5 \cdot 10^{-3}$ eV
Ar on Cu	20 keV	7354.8	0.0009	$4 \cdot 10^{-3}$ eV

The last column gives the energy transfers, corresponding to the lower limit of classical scattering (1.10).

From this table it is evident that the conditions for the applicability of classical mechanics fulfilled are in these cases.

According to Lindhard [11], the energy loss due to elastic collisions dominates, in the energy range considered in this thesis, over the inelastic energy loss, due to the stopping of moving atoms by the electrons of the solid target. Consequently, we shall not introduce this electronic stopping effect explicitly. Its effect will be supposed to be incorporated in the form of the inverse power potential, assumed for the inter-atomic interaction.

* * *
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CHAPTER II

RANGES OF PROJECTILES IN AMORPHOUS

Lindhard et al[11] have given a treatment of the total pathlength, travelled by a projectile in an amorphous target and they have also calculated first - and second - order moments of some range quantities. We shall generalize his treatment to higher - order moments of these latter quantities for the power - potential cross sections introduced in Chapter I.

Suppose a projectile starts with given kinetic energy E and a given direction of motion characterized by the unit vector $\vec{n}$ from a point inside the target material which we shall take as the origin of the co-ordinate system. This point can be identified with the point of entrance of the projectile into the target. We must keep in mind that the formalism which is developed in this chapter is based on a model in which the target material is infinitely extended through all space. We shall come back to this point later in this chapter. We begin our treatment with supposing the projectile to be of the same species as the target atoms and furthermore that the successive collisions undergone by the projectile are uncorrelated.

We introduce the probability density function $p(\vec{r},\vec{n},E)$ such that the probability that a projectile, starting from the origin with kinetic energy E and direction of motion $\vec{n}$, will come to rest in the element of volume $d\vec{r}$ around the point with vectorial co-ordinate $\vec{r}$ is given by $p(\vec{r},\vec{n},E)\,d\vec{r}$. Let the number of scattering centra per unit volume in the target be N. Then, if the projectile moves over a distance $\Delta\vec{r}$, immediately after the beginning of its journey, the probability that it will suffer within this distance a collision in which an energy between T and T + dT is transferred to a target atom and that it will be deflected over the corresponding scattering angle is given by $N\,|\Delta\vec{r}|\,d\sigma_1'$ (cf. (1.6)). After such a collision, it has the kinetic energy E - T, and its direction of motion is given by the unit vector $\vec{n}'$. Its probability to arrive in the chosen element of volume $d\vec{r}$ is then given by $p(\vec{r}-\Delta\vec{r},\vec{n}',E-T)\,d\vec{r}$. There is also the possibility that it will not be scattered while moving over the distance $\Delta\vec{r}$. The probability for this is $1-N\,|\Delta\vec{r}|\int_\Delta^E d\sigma'$ and the probability for arriving in $d\vec{r}$ is then given by $p(\vec{r}-\Delta\vec{r},\vec{n},E)\,d\vec{r}$. By combining these two possibilities and integrating over all possible energy transfers T, we obtain for p the following equation

$$p(\vec{r},\vec{n},E) = N\,|\Delta\vec{r}|\int_\Delta^E d\sigma'\,p(\vec{r}-\Delta\vec{r},\vec{n}',E-T) + \left(1-N\,|\Delta\vec{r}|\int_\Delta^E d\sigma'\right)p(\vec{r}-\Delta\vec{r},\vec{n},E) \tag{2.1}$$

A slight rearrangement gives

$$(2.2) \qquad \frac{p(\vec{r},\vec{n},E) - p(\vec{r}-\Delta\vec{r},\vec{n},E)}{|\Delta\vec{r}|} = N\int_{\Delta}^{E} d\sigma' \left[p(\vec{r}-\Delta\vec{r},\vec{n}',E-T) - p(\vec{r}-\Delta\vec{r},\vec{n},E) \right]$$

Because the targetmaterial is amorphous and since all scattering events have azimuthal symmetry $p(\vec{r},\vec{n},E)$ can only be a function of $r = |\vec{r}|$, E and $\eta = (\vec{r}.\vec{n})/r$, the cosine of the angle between the vector $\vec{r}$ and the initial direction of motion $\vec{n}$. This is shown in Fig. 1, where the angle φ_1 is the azimuthal co-ordinate of the volume element $d\vec{r} = r^2\, dr\, d\eta\, d\varphi_1$.

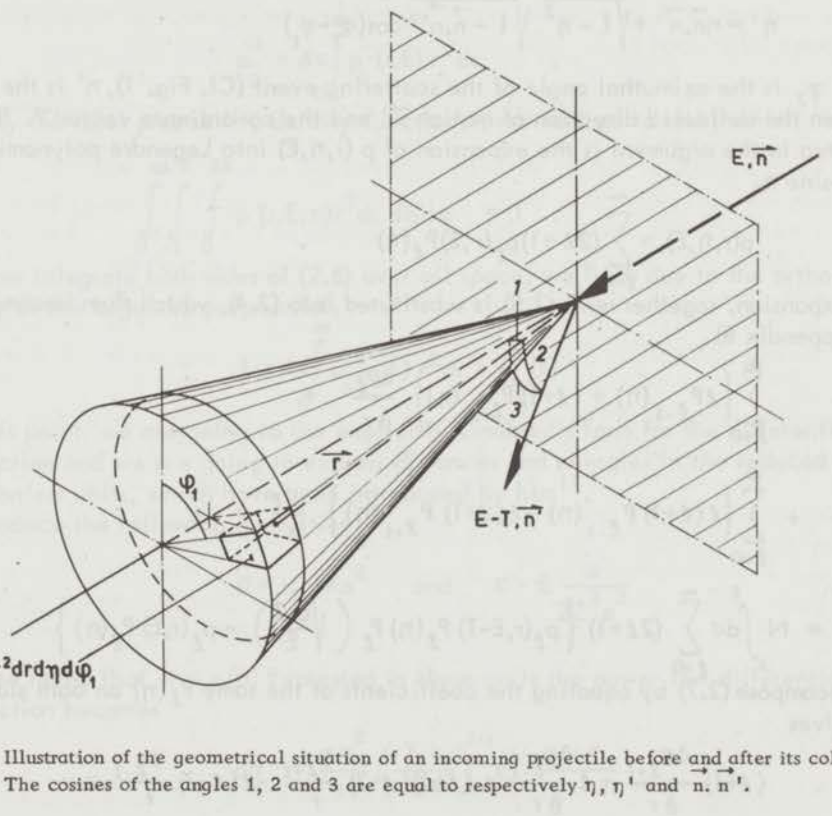

Fig. 1. Illustration of the geometrical situation of an incoming projectile before and after its collision. The cosines of the angles 1, 2 and 3 are equal to respectively η, η' and $\vec{n}.\vec{n}'$.

Hence

$$(2.3) \qquad p(\vec{r},\vec{n},E)\, d\vec{r} = p(r,\eta,E)\, r^2 dr\, d\eta\, d\varphi_1 \quad .$$

If we make use of this and take the limit $|\Delta\vec{r}| \rightarrow 0$, (2,2) becomes after a simple calculation

$$(2.4)\qquad \eta\,\frac{\partial p}{\partial r} + \frac{1-\eta^2}{r}\,\frac{\partial p}{\partial \eta} = N\int_{\Delta}^{E} d\sigma'\Big[\,p(r,\eta',E-T) - p(r,\eta,E)\Big] \quad .$$

The function $p(r,\eta,E)$ is supposed to be an analytic function of its variables. This implies that if we take the form (1.5) for $d\sigma'$ and (1.4) for $d\sigma$ the integral on the right-hand side of (2.4) converges in the limit $\Delta \to 0$ and we shall take that limit from now on.

According to the cosine rule of spherical trigonometry we can write

$$(2.5)\qquad \eta' = \eta\vec{n}.\vec{n}' + \sqrt{1-\eta^2}\,\sqrt{1-\vec{n}.\vec{n}'^2}\,\cos(\varphi_2-\varphi_1)$$

where φ_2 is the azimuthal angle of the scattering event (Cf. Fig. 1), η' is the angle between the deflected direction of motion $\vec{n}'$ and the co-ordinate vector $\vec{r}$. The next step in the argument is the expansion of $p(r,\eta,E)$ into Legendre polynomials of the cosine η,

$$(2.6)\qquad p(r,\eta,E) = \sum_{\ell=0}^{\infty} (2\ell+1)\,p_\ell(r,E)\,P_\ell(\eta) \quad .$$

This expansion, together with (2.5) is substituted into (2.4), which then becomes (cf. Appendix B)

$$(2.7)\qquad \sum_{\ell=0}^{\infty}\Big\{\ell P_{\ell-1}(\eta) + (\ell+1)P_{\ell+1}(\eta)\Big\}\,\frac{\partial p_\ell}{\partial r} \; +$$

$$+ \sum_{\ell=0}^{\infty}\Big\{\ell(\ell+1)P_{\ell-1}(\eta) - \ell(\ell+1)P_{\ell+1}(\eta)\Big\}\,\frac{p_\ell}{r} =$$

$$= N\int_{\Delta}^{E} d\sigma \sum_{\ell=0}^{\infty}(2\ell+1)\Big\{p_\ell(r,E-T)\,P_\ell(\eta)\,P_\ell\Big(\sqrt{\frac{E-T}{E}}\Big) - p_\ell(r,E)\,P_\ell(\eta)\Big\} \quad .$$

We decompose (2.7) by equating the coefficients of the same $P_\ell(\eta)$ on both sides. This gives

$$(\ell+1)\,\frac{\partial p_{\ell+1}}{\partial r} + \ell\,\frac{\partial p_{\ell-1}}{\partial r} + (\ell+1)(\ell+2)\,\frac{p_{\ell+1}}{r} - \ell(\ell-1)\,\frac{p_{\ell-1}}{r} =$$

$$(2.8)\qquad = N(2\ell+1)\int_0^E d\sigma\Big\{p_\ell(r,E-T)\,P_\ell\Big(\sqrt{\frac{E-T}{E}}\Big) - p_\ell(r,E)\Big\} \quad .$$

We can now introduce moments of different order of the range, which are defined as follows

$$(2.9)\qquad p_\ell^n(E) = 4\pi\int_0^\infty p_\ell(r,E)\,r^{n+2}\,dr \quad .$$

From this definition we can by multiplication of (2.8) with r^{2+n} and integration over r obtain the following recurrence relation between the different moments

$$(2.10)\qquad (\ell+1)(\ell-n)p^{n-1}_{\ell+1} - \ell(\ell+n+1)p^{n-1}_{\ell-1} = (2\ell+1)N\int_0^E d\sigma\left[p^n_\ell(E-T)\,P_\ell\left(\sqrt{\frac{E-T}{E}}\right) - p^n_\ell(E)\right]$$

Eq. (2.10) will be the starting point for the calculation of the different range quantities. Consider first the moment

$$(2.11)\qquad p^0_0 = 4\pi\int_0^\infty p_0\,(r,E)\,r^2\,dr \quad .$$

Evidently the total probability density function is normalized to unity which means that

$$(2.12)\qquad \int_0^\infty\int_{-1}^1\int_0^{2\pi} p\,(r,E,\eta)r^2 dr\,d\eta\,d\varphi_1 = 1 \quad .$$

If we now integrate both sides of (2.6) over all space, we find, due to the orthogonality of the Legendre polynomials

$$(2.13)\qquad 1 = 4\pi\int_0^\infty p_0\,(r, E)\,r^2 dr = p^0_0\,(E) \quad .$$

From this point, we are going to use explicitly Lindhard's form for the differential cross section and we are going to express distances and energies in the reduced dimensionless units, which have been introduced by him[11].
We introduce the following quantities

$$(2.14)\qquad \rho = r.N\pi a^2 \quad \text{and} \quad \varepsilon = E\,\frac{a}{2Z^2e^2} \quad .$$

It may be noted that $\varepsilon = a/b$. Expressed in these units the power law differential cross section becomes

$$(2.15)\qquad d\sigma = \frac{\pi a^2}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s} \varepsilon^{1/s}\,\frac{d\tau}{\tau^{1+1/s}}$$

where τ is the reduced transferred energy. Transforming r and E into ρ and ε in (2.4), we get with the help of (2.14) in the limit $\Delta \rightarrow 0$ the equation

$$(2.16)\qquad \eta\,\frac{\partial p}{\partial \rho} + \frac{1-\eta^2}{\rho}\,\frac{\partial p}{\partial \eta} = \frac{1}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s} \varepsilon^{1/s}\int_0^\varepsilon \frac{d\tau}{\tau^{1+1/s}}\,\delta\left(\vec{n}\,\vec{n}' - \sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\right)\frac{d\Omega'}{2\pi}\,\cdot$$
$$\cdot\left[p(\rho,\eta',\varepsilon-\tau) - p(\rho,\eta,\varepsilon)\right] \quad .$$

A straightforward argument now leads to the analog of (2.11) in reduced variables

$$(2.17)\qquad (\ell+1)(\ell-n)\, p^{n-1}_{\ell+1}(\varepsilon) - \ell(\ell+n+1)\, p^{n-1}_{\ell-1}(\varepsilon) =$$

$$= \frac{(2\ell+1)}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s} \varepsilon^{1/s}\int_0^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}}\left[p^n_{\ell}(\varepsilon-\tau)\, P_{\ell}\left(\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\right) - p^n_{\ell}(\varepsilon)\right]$$

where $p^n_{\ell}(\varepsilon) = 4\pi\int_0^{\infty} p_{\ell}(\rho,\varepsilon)\,\rho^{2+n}\, d\rho$. Of course again $p^0_0(\varepsilon) = 1$.

It will now be shown that from the recursion relation (2.17) it is possible to calculate all higher moments for which $(n+\ell)$ is even and $n \geqq \ell$.
Consider the equation for the moment $p^1_1(\varepsilon)$. From (3.17 we find that the equation for this moment is

$$(2.18)\qquad -3 = \frac{3}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}\varepsilon^{1/s}\int_0^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}\left[p^1_1(\varepsilon-\tau)\sqrt{\frac{\varepsilon-\tau}{\varepsilon}} - p^1_1(\varepsilon)\right].$$

To find the solution, we introduce the variable of integration, $y = \tau/\varepsilon$. (2.18) then becomes

$$(2.19)\qquad -1 = \frac{1}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}\int_0^{1}\frac{dy}{y^{1+1/s}}\left[p^1_1(\varepsilon-\tau)\sqrt{1-y} - p^1_1(\varepsilon)\right].$$

We try as a solution $p_1(\varepsilon) = \lambda\,\varepsilon^{2/s}$, where λ is independent of ε. Substitution into (2.18) yields for λ the equation

$$(2.20)\qquad -1 = \frac{1}{s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\lambda\int_0^{1}\frac{dy}{y^{1+1/s}}\left[(1-y)^{2/s+1/2} - 1\right]$$

from which follows

$$(2.21)\qquad \lambda = -\frac{1}{\dfrac{1}{s}\left(\dfrac{\gamma_s k_s}{2}\right)^{2/s}\displaystyle\int_0^{1}\frac{dy}{y^{1+1/s}}\left[(1-y)^{2/s+1/2} - 1\right]}$$

The integral in the denominator can be calculated by partial integration. The result becomes

$$(2.22)\qquad \lambda = \frac{1}{\left(\dfrac{\gamma_s k_s}{2}\right)^{2/s}\left[\left(2/s+1/2\right)B\left(1-1/s;\, 2/s+1/2\right) - 1\right]}\quad .$$

In order to prove the uniqueness of this solution, we substitute into (2.18) the function $p^*(\varepsilon) = p_1^1(\varepsilon) - \lambda\varepsilon^{2/s}$, where λ is given by (2.22). This results in the following equation for $p^*(\varepsilon)$

$$0 = \int_0^\varepsilon \frac{d\tau}{\tau^{1+1/s}} \left[p^*(\varepsilon-\tau)\sqrt{\frac{\varepsilon-\tau}{\varepsilon}} - p^*(\varepsilon) \right] .$$

Because we have supposed that $p(r,\eta,E)$ is an analytic function, it is easy to see from its definition that the moment $p_1^1(\varepsilon)$ is also analytic in ε and hence also $p^*(\varepsilon)$. Then it can be shown that the only possible form for $p^*(\varepsilon)$ is $p^*(\varepsilon) = a/\sqrt{\varepsilon}$ where a is a constant, from which follows $p_1^1(\varepsilon) = \lambda\varepsilon^{2/s} + a/\sqrt{\varepsilon}$. As the physical boundary condition, imposed on $p(\rho,\eta,\varepsilon)$ for $\varepsilon = 0$ implies that $p_1^1(0) = 0$, it follows that $a = 0$. This argument is valid for the integral equations for the higher moments, which are given hereafter as well.

The higher moments can be calculated in the same way. Take the moment $p_0^2(\varepsilon)$. Eq. (2.17) gives

$$(2.23) \qquad -2p_1^1(\varepsilon) = \frac{1}{s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s} \varepsilon^{1/s}\int_0^\varepsilon \frac{d\tau}{\tau^{1+1/s}}\left[p_0^2(\varepsilon-\tau) - p_0^2(\varepsilon)\right] .$$

We have found that $p_1(\varepsilon) = \lambda\varepsilon^{2/s}$. The procedure is precisely the same as in the preceding case, only now we put $p_0^2(\varepsilon) = k\varepsilon^{4/s}$. A straightforward calculation then gives

$$(2.24) \qquad k = \frac{2\lambda}{\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\left[{}^4/_s\, B(1-{}^1/_s;\, {}^4/_s) - 1\right]} .$$

For the moment $p_2^2(\varepsilon)$ we find from (2.17)

$$(2.25) \qquad -10p_1^1(\varepsilon) = \frac{5}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s} \varepsilon^{1/s}\int_0^\varepsilon \frac{d\tau}{\tau^{1+1/s}}\left[p_0^2(\varepsilon-\tau)\left(\frac{3}{2}\,\frac{\varepsilon-\tau}{\varepsilon} - \frac{1}{2}\right) - p_2^2(\varepsilon)\right]$$

We try the solution $p_2^2(\varepsilon) = \mu\varepsilon^{4/s}$ and find for μ

$$(2.26) \qquad \mu = \frac{2}{\left(\frac{\gamma_s k_s}{2}\right)^{2/3}\left[\frac{3}{2}\left(\frac{4}{s}+1\right) B(1-{}^1/_s;\, {}^4/_s+1) - {}^2/_s\, B(1-{}^1/_s;\, {}^4/_s) - 1\right]}$$

In the same way all higher moments with $n+\ell$ even and $n \geqq \ell$ can be found. In general such moments $p_\ell^n(\varepsilon)$ are proportional to $\varepsilon^{2n/s}$.

We shall now show how this calculation can be adapted to the case that the projectile differs in species from the target material. In that case the projectile has charge number and mass respectively Z_1 and m_1 and the target atoms Z_2 and m_2. Lindhard's expression for the differential cross section with angular distribution for this case is given by (1.5), where the factor

$$\delta\left(\overleftrightarrow{nn''} - \frac{m_1+m_2}{2\sqrt{m_1 m_2}}\sqrt{T/E}\right)\frac{d\Omega''}{2\pi}$$

can be dropped, because the hit particle is not considered in this calculation and the corresponding variables do not occur in the quantities to be calculated.

It is evident that the argument, leading to Eq. (2.2) remains valid, except that we must write γE instead of E in the upper limit of the integral. As before, the probability density p is a function only of r, η and E, so an expansion into Legendre polynomials is again possible. Finally for the moments $p_\ell^n(E)$ we arrive at the equation

$$(2.27)\qquad (\ell+1)(\ell-n)\,p_{\ell+1}^{n-1}(E) - \ell(\ell+n+1)\,p_{\ell-1}^{n-1}(E) =$$

$$= (2\ell+1)N\int_\Delta^{\gamma E} d\sigma\left[p_\ell^n(E-T)\,P_\ell\left(\frac{m_1+m_2}{2m_1}\sqrt{\frac{E-T}{E}} + \frac{m_1-m_2}{2m_1}\sqrt{\frac{E}{E-T}}\right) - p_\ell^n(E)\right]$$

by carrying out the same operations as for (2.10). (Cf. Appendix B). As before we take the limit $\Delta \to 0$. We make the transformation[11]

$$(2.28)\qquad \rho = N\pi a^2\gamma . r \quad\text{and}\quad \varepsilon = \frac{a m_2}{Z_1 Z_2 e^2 (m_1+m_2)} . E = \frac{a}{b} .$$

The generalization of (2.17) is then

$$(2.29)\qquad (\ell+1)(\ell-n)\,p_{\ell+1}^{n-1}(\varepsilon) - \ell(\ell+n+1)\,p_{\ell-1}^{n-1}(\varepsilon) =$$

$$= \frac{(2\ell+1)}{\gamma . s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}(\gamma\varepsilon)^{1/s}\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}\left[p_\ell^n(\varepsilon-\tau)\,P_\ell\left(\frac{m_1+m_2}{2m_1}\sqrt{\frac{\varepsilon-\tau}{\varepsilon}} + \frac{m_1-m_2}{2m_1}\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\right) - p_\ell^n(\varepsilon)\right] .$$

Of course again $p_0^0(\varepsilon) = 1$. The equation for $p_1^1(\varepsilon)$ reads

$$(2.30)\qquad -3 = \frac{3}{\gamma s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}(\gamma\varepsilon)^{1/s}\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}\left[p_1^1(\varepsilon-\tau)\left\{\frac{m_1+m_2}{2m_1}\sqrt{\frac{\varepsilon-\tau}{\varepsilon}} + \frac{m_1-m_2}{2m_1}\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\right\} - p_1^1(\varepsilon)\right] .$$

This is again a linear integral equation which is solved by substituting the solution $p_1^1(\varepsilon) = \lambda'\,\varepsilon^{2/s}$ and introducing the variable of integration $y = \tau/\gamma\varepsilon$. The factor λ' can be calculated with the result

$$(2.31)\qquad \lambda' = \Bigg[\frac{1}{\gamma}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\Bigg\{\frac{m_1+m_2}{2m_1}(1-\gamma)^{2/s+1/2} + \frac{m_1-m_2}{2m_1}(1-\gamma)^{2/s-1/2} - 1 + \gamma^{1/s}\left(\frac{m_1+m_2}{2m_1}\left(^2/s+^1/2\right) B_\gamma\left(1-^1/s; ^2/s+^1/2\right) + \frac{m_1-m_2}{2m_1}\left(^2/s-^1/2\right) B_\gamma\left(1-^1/s; ^2/s-^1/2\right) - 1\right)\Bigg\}\Bigg]^{-1}$$

In this formula B_γ denotes the incomplete Beta function[17].
The calculation of the higher moments proceeds as in the case of equal mass. All the p^n_ℓ with $n \geqq \ell$ and $n+\ell$ even can be determined from (2.27).

We shall now give a geometrical interpretation of the different moments.
From the preceding argument it is clear that $p_0^0(\varepsilon)$ is nothing but the probability of finding the projectile anywhere in space after it has completed its journey (cf.(2.13)).
The meaning of the moment $p_1^1(\varepsilon)$ can be found from (2.3) and (2.6), expressed in reduced units. To obtain it, we multiply both members of (2.6) with $\rho . P_1(\eta) = \rho\eta$ and then integrate over all space. Using the orthogonality property of the P_ℓ, the result is

$$(2.32)\qquad \overline{\rho\eta} = 4\pi\int_0^\infty p\,(\rho,\varepsilon)\,\rho^3\,d\rho = p_1^1(\varepsilon) \quad .$$

Hence $p_1^1(\varepsilon)$ is the average of the projection of the distance ρ from the origin, reached by the projectile, on its initial direction of motion. Following Lindhard and co-workers, we shall call this quantity $\overline{\rho_p}$.
We obtain the interpretation of $p_0^2(\varepsilon)$ by multiplying both sides of (2.6) with $\rho^2 = \rho^2 P_0(\eta)$ and again integrating over all space. The result is

$$(2.33)\qquad \overline{\rho^2} = 4\pi\int_0^\infty p_0\,(\rho,\varepsilon)\,\rho^4\,d\rho = p_0^2(\varepsilon) \quad .$$

So $p_0^2(\varepsilon)$ is the average square of the distance from the origin, reached by the projectile. In the same way an expression for $p_2^2(\varepsilon)$ can be found by multiplying (2.7) with $\rho^2 P_2(\eta) = \rho^2(3/2\,\eta^2 - \frac{1}{2})$ and integrating. This time the result is

$$(2.34)\qquad ^3/2\;\overline{\rho^2\eta^2} - \tfrac{1}{2}\overline{\rho^2} = \overline{\rho_p^2} - \tfrac{1}{2}\overline{\rho_\perp^2} = p_2^2(\varepsilon)$$

$\rho_\perp$ is defined by $\rho_\perp = \rho\sqrt{1-\eta^2}$ and can be geometrically interpreted as the projection of the distance ρ from the origin, reached by the projectile on the plane, perpendicular to $\vec{n}$. From Eqs. (2.33) and (2.34) $\overline{\rho_p^2}$ and $\overline{\rho_\perp^2}$ can be found separately, because obviously $\overline{\rho^2} = \overline{\rho_p^2} + \overline{\rho_\perp^2}$ (Cf. Fig. 2).

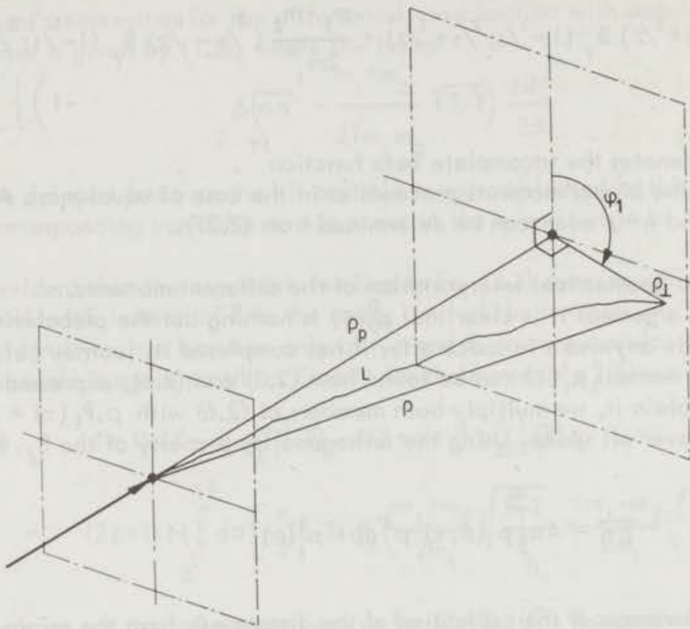

Fig. 2 Illustration of the geometrical meaning of ρ, ρ_p and $\rho_\perp$ as introduced in the text. L denotes the total length of the path, travelled by the projectile.

In this way all higher moments $p_\ell^n(\varepsilon)$ with $n + \ell$ even and $n \geqq \ell$ can be calculated and interpreted. A table of all moments up to 5^{th} order will now be given and conversely the expressions of all moments of ρ_p up to 5^{th} order in the moments $p_\ell^n(\varepsilon)$

$$p_0^0(\varepsilon) = 1$$
$$p_1^1(\varepsilon) = \overline{\rho_p}$$
$$p_0^2(\varepsilon) = \overline{\rho_p^2} + \overline{\rho_\perp^2}$$
$$p_2^2(\varepsilon) = \overline{\rho_p^2} - \tfrac{1}{2}\overline{\rho_\perp^2}$$
$$p_1^3(\varepsilon) = \overline{\rho_p^3} + \overline{\rho_p \rho_\perp^2}$$
$$p_3^3(\varepsilon) = \overline{\rho_p^3} - \tfrac{3}{2}\overline{\rho_p \rho_\perp^2}$$
$$p_0^4(\varepsilon) = \overline{\rho_p^4} + 2\,\overline{\rho_p^2 \rho_\perp^2} + \overline{\rho_\perp^4}$$
$$p_2^4(\varepsilon) = \overline{\rho_p^4} + \tfrac{1}{2}\overline{\rho_p^2 \rho_\perp^2} - \tfrac{1}{2}\overline{\rho_\perp^4}$$
$$p_4^4(\varepsilon) = \overline{\rho_p^4} - 3\,\overline{\rho_p^2 \rho_\perp^2} + \tfrac{3}{8}\overline{\rho_\perp^4}$$
$$p_1^5(\varepsilon) = \overline{\rho_p^5} + 2\,\overline{\rho_p^3 \rho_\perp^2} + \overline{\rho_p \rho_\perp^4}$$
$$p_3^5(\varepsilon) = \overline{\rho_p^5} - \tfrac{1}{2}\overline{\rho_p^3 \rho_\perp^2} - \tfrac{3}{2}\overline{\rho_p \rho_\perp^4}$$
$$p_5^5(\varepsilon) = \overline{\rho_p^5} - 5\,\overline{\rho_p^3 \rho_\perp^2} + \tfrac{15}{8}\overline{\rho_p \rho_\perp^4}$$

and conversely

$$\overline{\rho_p} = p_1^1(\varepsilon)$$
$$\overline{\rho_p^2} = \frac{p_0^2(\varepsilon) + 2\,p_2^2(\varepsilon)}{3}$$
$$\overline{\rho_p^3} = \frac{3\,p_1^3(\varepsilon) + 2\,p_3^3(\varepsilon)}{5}$$
$$\overline{\rho_p^4} = \frac{7\,p_0^4(\varepsilon) + 20\,p_2^4(\varepsilon) + 8\,p_4^4(\varepsilon)}{35}$$
$$\overline{\rho_p^5} = \frac{33.75\,p_1^5(\varepsilon) + 35\,p_3^5(\varepsilon) + 10\,p_5^5(\varepsilon)}{78.75}$$

For the case that $s = 2$ (inverse square potential) it is clear from these results that $\overline{\rho_p^n} \sim \varepsilon^n$ for every n.

The generalization of the preceding theory for the case of a mixture of two kinds of atoms is straightforward. Suppose, we have a chemical compound A_pB_q. The differential cross section for collisions of a projectile which is either an A- or a B-atom we denote by $d\sigma_A$ and $d\sigma_B$, where

$$(2.35^a)\qquad d\sigma_A = \frac{\pi}{s}\left(\frac{b_A^2}{4}\, a_A^{2s-2}\, k_s^2 \gamma_s^2\, T_A\right)^{1/s} \frac{dT}{T^{1+1/s}} = \frac{\pi a_A^2}{s}\left(\frac{\gamma_s k_s}{2\varepsilon_A}\right)^{2/s} \frac{dy}{y^{1+1/s}}$$

and

$$(2.35^b)\qquad d\sigma_B = \frac{\pi}{s}\left(\frac{b_B^2}{4}\, a_B^{2s-2}\, k_s^2 \gamma_s^2\, T_B\right)^{1/s} \frac{dT}{T^{1+1/s}} = \frac{\pi a_B^2}{s}\left(\frac{\gamma_s k_s}{2\varepsilon_B}\right)^{2/s} \frac{dy}{y^{1+1/s}}$$

We have supposed here that the exponent s is the same for the interaction of the projectile with A- and B-atoms. Furthermore b_A and b_B are Bohr's collision diameters for collisions of the projectile with A- and B-atoms, respectively, a_A and a_B are the corresponding screening lengths and $T_A = \gamma_A E$ and $T_B = \gamma_B E$ with

$$\gamma_{A,B} = \frac{4\, m_1 \cdot m_{A,B}}{(m_1 + m_{A,B})^2}$$

Finally

$$(2.36^a)\qquad \varepsilon_A = \frac{a_A m_A}{Z_{pr} Z_A e^2 (m_1 + m_A)}\, E = \frac{a_A}{b_A}$$

and

$$(2.36^b)\qquad \varepsilon_B = \frac{a_B m_B}{Z_{pr} Z_B e^2 (m_1 + m_B)}\, E = \frac{a_B}{b_B}$$

and in (2.35^a) $y = T/T_A$ and in (2.35^b) $y = T/T_B$.

It is now again possible to write down an equation for the probability density function $p(\vec{r}, \vec{n}, E)$. Suppose the projectile moves over a distance $\Delta \vec{r}$ after beginning its journey. The density of the amorphous target material is N such that there are $pN/p+q$ A-atoms and $qN/p+q$ B-atoms per unit volume. The probability that it suffers within $\Delta\vec{r}$ collision in which energy between T and T+dT is transferred to a target atom is equal to

$$N|\Delta\vec{r}|\left\{\frac{p}{p+q}\, d\sigma_A + \frac{q}{p+q}\, d\sigma_B\right\}$$

and the probability that it does not collide in $\Delta\vec{r}$ is

$$1 - N|\Delta\vec{r}|\left\{\frac{p}{p+q}\int_{\Delta}^{T_A} d\sigma_A + \frac{q}{p+q}\int_{\Delta}^{T_B} d\sigma_B\right\}$$

This enables us to write down the following generalization for the general range equation

$$(2.37)\qquad p(\vec{r},\vec{n},E) = N|\Delta\vec{r}|\left\{\frac{p}{p+q}\int_{\Delta}^{T_A} d\sigma'_A \,.\, p(\vec{r}-\Delta\vec{r},\vec{n}',E-T) + \frac{q}{p+q}\int_{\Delta}^{T_B} d\sigma'_B \,.\, p(\vec{r}-\Delta\vec{r},\vec{n}',E-T)\right\} + \left(1-N|\Delta\vec{r}|\left(\frac{p}{p+q}\int_{\Delta}^{T_A} d\sigma'_A + \frac{q}{p+q}\int_{\Delta}^{T_B} d\sigma'_B\right)\right) p(\vec{r}-\vec{r},\vec{n},E)$$

$d\sigma'_A$ and $d\sigma'_B$ denote differential cross sections with the angular distribution after scattering included (cf. (1.5)). From this point the procedure is precisely the same as described in the earlier part of this chapter, i.e. use is made of the fact that due to the amorphous nature of the target, the function $p(\vec{r},\vec{n},E)$ depends only on $r, \eta = (\vec{n}\,.\,\vec{r})/r$ and E and that it is an analytic function.
$p(r,\eta,E)$ is expanded in Legendre polynomials $P_\ell(\eta)$, which expansion is substituted into (2.37), after this has been rearranged in the form of (2.2). Next the coefficients of the same $P_\ell(\eta)$ are equated on both sides and the spatial moments $p_\ell^n(E) = 4\pi\int_0^\infty p(r,E)\, r^{n+2}\, dr$ are introduced. After all these operations have been carried out, we are left with the recursion relation

$$(2.38)\qquad (\ell+1)(\ell-n)\, p_{\ell+1}^{n-1}(E) - \ell(\ell+n+1)\, p_{\ell-1}^{n-1}(E) =$$

$$= (2\ell+1)\, N\frac{p}{p+q} C_A\int_0^{T_A}\frac{dT}{T^{1+1/s}}\left[p_\ell^n(E-T)\, P_\ell\left(\sqrt{\frac{E-T}{E}}\,\frac{m_1+m_A}{2m_1}+\sqrt{\frac{E}{E-T}}\,\frac{m_1-m_A}{2m_1}\right)-p_\ell^n(E)\right] +$$

$$+ (2\ \ +1)\, N\frac{q}{p+q} C_B\int_0^{T_B}\frac{dT}{T^{1+1/s}}\left[p_\ell^n(E-T)\, P_\ell\left(\sqrt{\frac{E-T}{E}}\,\frac{m_1+m_B}{2m_1}+\sqrt{\frac{E}{E-T}}\,\frac{m_1-m_B}{2m_1}\right)-p_\ell^n(E)\right]$$

where we have taken the limit $\Delta \to 0$.
Here C_A and C_B are the factors with which $dT/T^{1+1/s}$ is multiplied in (2.35^a) and (2.35^b) and m_1, m_A and m_B respectively the masses of projectile, A- and B-atoms. As has been shown, the entire formalism can be expressed in reduced variables ρ and ε, but attention must now be paid to one point, namely that we have two kinds of target atoms and consequently two possible choices of ρ and ε. It is easy to overcome this difficulty. We make the transformation

$$(2.39)\qquad \rho = N\pi a_A^2\gamma_A\,.\,r \quad\text{and}\quad \varepsilon = \frac{a_A m_A}{Z_A Z_1 e^2(m_A+m_1)}\,.\,E$$

where $\gamma_A = \dfrac{4m_1 m_A}{(m_1+m_A)^2}$.

If we now put $\varepsilon_B = f\varepsilon$ and $a_B = ga$, the recurrence relation can be expressed in reduced variables

(2.40) $$(\ell+1)(\ell-n)\,p^{n-1}_{\ell+1}(\varepsilon) - \ell(\ell+n+1)\,p^{n-1}_{\ell-1}(\varepsilon) =$$

$$= (2\ell+1)\frac{p}{p+q}\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2\varepsilon_A}\right)^{2/s}\int_0^1 \frac{dy}{y^{1+1/s}}\left[p^n_\ell(\varepsilon-\tau)\,P_\ell\left(\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\frac{m_1+m_A}{2m_1}+\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\frac{m_1-m_A}{2m_1}\right)-p^n_\ell(\varepsilon)\right]$$

$$+(2\ell+1)\frac{q}{p+q}\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2f\varepsilon_A}\right)^{2/s} g^2\int_0^1 \frac{dy}{y^{1+1/s}}\left[p^n_\ell(\varepsilon-\tau)P_\ell\left(\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\frac{m_1+m_B}{2m_1}+\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\frac{m_1-m_B}{2m_1}\right)-p^n_\ell(\varepsilon)\right]$$

In the first integral $y = \dfrac{T}{T_A} = \dfrac{\tau}{\gamma_A\varepsilon}$ and in the second one $y = \dfrac{T}{T_B} = \dfrac{\tau}{\gamma_B\varepsilon}$.

Of course $p^0_0(\varepsilon) = 1$. Consider the equation for the moment p^1_1. This reads

$$-1 = \frac{p}{p+q}\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2\varepsilon_A}\right)^{2/s}\int_0^1 \frac{dy}{y^{1+1/s}}\left[p^1_1(\varepsilon-\tau)\left\{(1-\gamma_A y)^{\frac{1}{2}}\frac{m_1+m_A}{2m_1}+(1-\gamma_A y)^{-\frac{1}{2}}\frac{m_1-m_A}{2m_1}\right\}-p^1_1(\varepsilon)\right]$$

(2.41)
$$+\frac{q}{p+q}\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2f\varepsilon_A}\right)^{2/s} g^2\int_0^1 \frac{dy}{y^{1+1/s}}\left[p^1_1(\varepsilon-\tau)\left\{(1-\gamma_B y)^{\frac{1}{2}}\frac{m_1+m_B}{2m_1}+(1-\gamma_B y)^{-\frac{1}{2}}\frac{m_1-m_B}{2m_1}\right\}-p^1_1(\varepsilon)\right]$$

As before we try the solution $p^1_1(\varepsilon) = \alpha^1_1\varepsilon^{2/s}$. Substitution into (2.40) yields an equation for α^1_1, of which the solution is

$$\alpha^1_1 = \left[\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\frac{p}{p+q}\int_0^1\frac{dy}{y^{1+1/s}}\left\{\frac{m_1+m_A}{2m_1}(1-\gamma_A y)^{2/s+1/2}+\frac{m_1+m_A}{2m_1}(1-\gamma_A y)^{2/s-1/2}-1\right\}\right.$$

(2.42)
$$\left.+\frac{1}{s\gamma_A}\left(\frac{\gamma_s k_s}{2f}\right)^{2/s} g^2\frac{q}{p+q}\int_0^1\frac{dy}{y^{1+1/s}}\left\{\frac{m_1+m_B}{2m_1}(1-\gamma_B y)^{2/s+1/2}+\frac{m_1+m_B}{2m}(1-\gamma y)^{2/s-1/2}-1\right\}\right]^{-1}$$

The integrals converge at the lower limit and may by partial integration be reduced to incomplete B-functions. Evidently the higher moments can be found in the same way as before. In the equation for $p^n_\ell(\varepsilon)$ ($n \geqq \ell$ and $n+\ell$ even), which is obtained from (2.40), the substitution $p^n_\ell(\varepsilon) = \alpha^n_\ell\varepsilon^{2n/s}$, immediately yields an equation for α^n_ℓ in

terms of the proportionality factors of the lower-order moments, which have already been calculated. We then know the range moments $p_\ell^n(\varepsilon)$ as functions of the energy ε. The uniqueness of the solution may be proved in the same way as was done in the case of (2.19).
This calculation has been carried out for the case of ^{85}Kr-ions of various energies on Al_2O_3, which has been measured by Domey et al.[18]. They have bombarded amorphous targets with ions of different kinetic energies, of which one consisted of Al_2O_3, and was bombarded with ^{85}Kr. The direction of incidence of the projectiles was always normal to the surface. The technique was as follows.

A layer of oxyde has been formed anodically on the surface of a metal foil. It is then bombarded with a monoenergetic beam of radioactive ions of normal incidence. The activity of the target is measured after the bombardment. Then the oxyde layer is dissolved and the activity is measured again. Repeating this experiment for different thicknesses of the oxyde layer produces a curve which gives the fraction of the projectiles transmitted through the layer as a function of its thickness.

Let us call $f(\varepsilon,\rho_p)d\rho_p$ the probability that an ion with reduced initial kinetic energy ε will have a penetration depth between ρ_p and $\rho_p + d\rho_p$. The curve, measured by Domey et al, then represents in our formalism the quantity $1-\int_{-\infty}^{a} f(\varepsilon,\rho_p)\, d\rho_p$, as a function of a, where a is the thickness of the oxyde layer, expressed in reduced units. The appearence of $-\infty$ in the lower limit of the integral is a consequence of the fact that the theoretical model represents an ion starting at a given point in a given direction in target material which is infinitely extended through all space. The penetration depth could therefore conceivably be negative. In the actual experiment this would correspond with the case that a projectile is reflected out of the target material. It will turn out that the influence of this probability is negligible.

All moments up to 5^{th} order have been calculated for s = 2, which means that all $p_\ell^n(\varepsilon)$ are proportional to ε^n. All integrals, occurring in the expressions for the coefficients α_ℓ^n have been calculated numerically on an electronic computer. From the moment $p_\ell^n(\varepsilon)$ the moments up to 5^{th} order of the reduced penetration depth have been calculated with the help of the formulas, resulting from the geometrical interpretation of the $p_\ell^n(\varepsilon)$.

The factor k_s has been fitted to the experimentally measured value of the first-order moment, i.e. the average penetration depth, as given in ref. 18. The authors express the measured distances in units of $\mu g/cm^2$ which in the case of Al_2O_3 corresponds to 25.2 Å. In dimensionless units as given by (2.39), referred to the system Kr-Al, it means that with 1 $\mu g/cm^2$ there corresponds a distance $\rho = 0.0907$.

We consider three different values of the initial energy E of the ^{85}Kr-ions, 40, 80 and 160 keV. In every case the constant k_s is fixed by equating the theoretical expression for $p_1^1(\varepsilon)$ with the experimental value of the mean penetration depth. It is calculated by multiplying α_1^1 as given by (2.42) where $1 \equiv {}^{85}Kr$, $A \equiv Al$ and $B \equiv O$, with the corresponding value of ε and equating this to the experimental mean penetration depth, expressed in reduced units. The reduced energies ε, the experimental values of the average penetration depth and the resulting value of k_s are for these three cases given in the following table.

E (keV)	ε	R_p ($\mu g/cm^2$)	ρ_p	k_s
40	0.164	6.2	0.562	0.826
80	0.328	10.7	0.970	0.958
160	0.656	20.4	1.850	1

From the different moments of ρ_p an approximate cumulative distribution function for ρ_p can be constructed with the help of an Edgeworth asymptotic expansion[19], which has also been used by Baroody[12] in his range calculation. By a cumulative distribution function F(x) we mean a function which denotes the probability that a random variable X will be smaller than or equal to x, where $F(\infty) = 1$ and $F(-\infty) = 0$. That such a cumulative distribution function (c.d.f) provides an adequate description of the measured behaviour of the incoming projectiles follows from the set-up of the experiment. What is measured are the fractions of the projectiles which have not been stopped by layers of aluminium oxide of different thicknesses. In terms of a c.d.f. this corresponds with $1 - F(x)$, where x is a measure for the thickness of the oxide layer.
The Edgeworth form for the c.d.f. is as follows:

$$(2.43)\qquad F(x) \propto P(x) - \left[\frac{\gamma_1}{6} Z^{(2)}(x)\right] + \left[\frac{\gamma_2}{24} Z^{(3)}(x) + \frac{\gamma_1^2}{75} Z^{(5)}(x)\right] -$$

$$- \left[\frac{\gamma_3}{120} Z^{(4)}(x) + \frac{\gamma_1\gamma_2}{144} Z^{(6)}(x) + \frac{\gamma_1^3}{1296} Z^{(8)}(x)\right] + \text{higher terms.}$$

In this formula $x = \dfrac{\rho_p - \overline{\rho_p}}{\sqrt{\overline{\rho_p^2} - \overline{\rho}_p^2}}$, P(x) is the Gaussian c.d.f.

$P(x) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{x} e^{-t^2/2}\, dt$, $Z^{(n)}$ is the n^{th} derivative of the Gaussian normal curve $Z(x) = \dfrac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$ and γ_1, γ_2 and γ_3 are the following

expression in the moments

$$(2.44^a)\qquad \gamma_1 = (\overline{\rho_p^3} - 3\,\overline{\rho_p^2}\,\overline{\rho}_p + 2\overline{\rho}_p^3) \,/\, (\overline{\rho_p^2} - \overline{\rho}_p^2)^{3/2}$$

$$(2.44^b)\qquad \gamma_2 = (\overline{\rho_p^4} - 4\overline{\rho_p^3}\,\overline{\rho}_p - 3\overline{\rho_p^2}^{\,2} + 12\,\overline{\rho_p^2}\,\overline{\rho}_p^2 + 6\overline{\rho}_p^4) / (\overline{\rho_p^2} - \overline{\rho}_p^2)^2$$

$$(2.44^c)\ \gamma_3 = \frac{(\overline{\rho_p^5} - 5\overline{\rho_p^4}\bar{\rho}_p - 10\overline{\rho_p^3}\,\overline{\rho_p^2} + 20\overline{\rho_p^3}\bar{\rho}_p^2 + 30\overline{\rho_p^2}\bar{\rho}_p^2 - 60\overline{\rho_p^2}\bar{\rho}_p^3 + 24\bar{\rho}_p^5)}{(\overline{\rho_p^2} - \bar{\rho}_p^2)^{5/2}}$$

The function F(x) has been calculated for those values of ρ_p , which corresponds with the thicknesses of the oxide layers, measured by Domey c.s. and for incoming energies of 40, 80 and 160 keV.

The comparison between theoretical and experimental results is shown in Fig. 3, from which the conclusion may be drawn that the correspondence between theory and experiment is quite satisfactory.

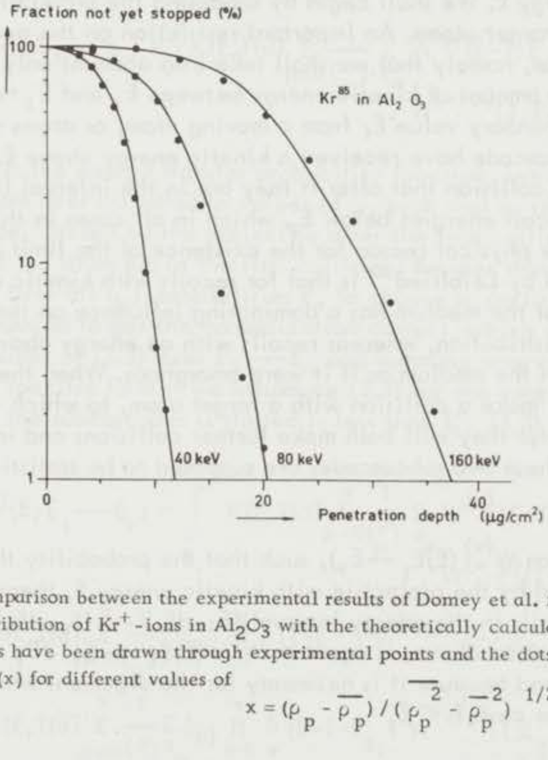

Figure 3. Comparison between the experimental results of Domey et al. for the penetration depth distribution of Kr^+-ions in Al_2O_3 with the theoretically calculated c.d.f. (2.43). The lines have been drawn through experimental points and the dots represent calculated values of F(x) for different values of

$$x = (\rho_p - \overline{\rho_p}) / (\overline{\rho_p^2} - \overline{\rho_p}^2)^{1/2} .$$

The variation in the factor k_s in the cross section for different energies may be interpreted as the influence of the change of the inelastic energy loss to atomic electrons for different energies of the projectiles.

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CHAPTER III

ON THE NUMBER OF LOW-ENERGY RECOILS IN A COLLISION CASCADE

In this chapter the supposition that the target material is amorphous will be dropped. Instead, we shall suppose that it has a poly- or mono-crystalline structure. The quantity which will be calculated in this chapter is the so-called collision density, denoted by $\overline{\nu}\,(E;E_1)$ and defined as follows.

$\overline{\nu}(E;E_1)\,dE_1$ is the average number of recoils in the energy interval between E_1 and E_1+dE_1, which are created in the course of a collision cascade, started by a projectile with kinetic energy E. We shall begin by supposing the projectile to be of the same species as the target atoms. An important restriction on the average recoil number must still be made, namely that we shall take into account only stationary atoms, which receive an amount of kinetic energy between E_1 and E_1+dE_1 where E_1 lies below a given boundary value E_f from a moving atom, or atoms which in the course of the collision cascade have received a kinetic energy above E_f and then lose so much in a single collision that after it they are in the interval (E_1, dE_1). We are interested only in recoil energies below E_f, which in all cases in this thesis is much smaller than E. The physical reason for the existence of the limit E_f, which has first been introduced by Leibfried[20] is that for recoils with kinetic energy below E_f the lattice structure of the medium has a dominating influence on the further energy and momentum distribution, whereas recoils with an energy above E_f are supposed to interact with the medium as if it were amorphous. When the projectile enters the target, it will make a collision with a target atom, to which it will transfer an energy T. Thereafter they will both make further collisions and in this way start two subcascades. These two subcascades are supposed to be statistically independent.

We introduce the function $W^{(\nu)}\,(E;E_1 -- E_\nu)$, such that the probability that, in the collision cascade, started by the projectile with kinetic energy E, there will be created precisely ν recoils in the energy interval $(E_1, dE_1) --- (E_\nu, dE_\nu)$ respectively with the restriction described above, is equal to $W^{(\nu)}\,(E;E_1 --- E_\nu)\,dE_1 --- dE_\nu$. In view of this restriction and because it is necessary for the argument which follows we must state that for the case $T < E_f$

$$W^{(\nu)}\,(T;E_1 --- E_\nu) = \delta_{\nu 1} \prod_{i=1}^{\nu} \delta(T-E_i) \tag{3.1}$$

We shall give an explanation of this formula.
If a recoil in the collision cascade has an energy $T \leqq E_f$ it cannot create any additional recoils and the only way it can contribute to the recoils $E_1 --- E_\nu$ created by the projectile with probability $W^{(\nu)}\,(E;E_1 --- E_\nu)$ is by being itself one of those recoils. Hence the Kronecker δ , indicating that the contribution can consist of only

one recoil. The Dirac δ-functions then fix its energy on one of the prescribed values.

The next point which must be discussed is the normalization of $W^{(\nu)}$. It is normalized according to

$$\sum_{\nu} \int_{\Delta}^{E} W^{(\nu)}(E;E_1 --- E_\nu)\, dE_1 --- dE_\nu = 1 . \tag{3.2}$$

This means that the sum of the probabilities for any number of recoils with any energy value between Δ and E_f in the cascade must necessarily be equal to 1.

It is clear that $W^{(\nu)}(E;E_1 --- E_\nu)$ is a symmetric function of $E_1 --- E_\nu$.
In view of the statistical independence of the two subcascades we can write for $W^{(\nu)}(E;E_1 --- E_\nu)$ the following equation

$$W^{(\nu)}(E;E_1 --- E_\nu) = \int_{\Delta}^{E} K(E,T)dT \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} W^{(\mu)}(E-T;E_{\alpha_1} --- E_{\alpha_\mu}) . \; W^{(\nu-\mu)}(T;E_{\alpha_{\mu+1}} --- E_{\alpha_\mu}) \quad . \tag{3.3}$$

Here K (E,T) is the energy transfer probability function, introduced in Chapter I. We have to sum over all possible values of μ, such that μ recoils are created by the subcascade, caused by the projectile after the first collision and $\nu-\mu$ by the subcascade of the atom hit in the first collision. Besides that we must then also, for every μ, sum over all $\binom{\nu}{\mu}$ possibilities P_α to choose μ particles out of ν. The factor $\binom{\nu}{\mu}^{-1}$ is introduced to get the normalization correct, which can be checked by integrating both sides of (3.3) over $E_1 --- E_\nu$ and summing over ν. Equation (3.3) can be given a more specific form if we introduce (3.1) for the case that the energy with which one of the subcascades is started is less then E_f. (3.3) then becomes

$$\begin{aligned} W^{(\nu)}(E;E_1 --- E_\nu) = & \int_{E_f}^{E-E_f} K(E,T)dT \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} W^{(\mu)}(E-T;E_{\alpha_1} --- E_{\alpha_\mu}) . \; W^{(\nu-\mu)}(T;E_{\alpha_{\mu+1}} --- E_{\alpha_\nu}) \; + \\ & + \int_{\Delta}^{E_f} K(E,T)dT \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P} \delta_{\mu 1} \prod_{i=1}^{\nu} \delta(T-E_{\alpha_1})\, W^{(\nu-\mu)}(E-T;E_{\alpha_{\mu+1}} --- E_{\alpha_\nu}) \; + \\ & + \int_{E-E_f}^{E} K(E,T)dT \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} \delta_{\mu 1} \prod_{i=1}^{\nu} \delta(E-T-E_{\alpha_1})\, W^{(\nu-\mu)}(T;E_{\alpha_{\mu+1}} --- E_{\alpha_\nu}) \quad . \end{aligned} \tag{3.4}$$

The last two terms on the right-hand side of (3.4) represent the probability that respectively the target atom or the projectile comes directly in one of the energy intervals $(E_{\alpha_i}, dE_{\alpha_i})$ as a result of the first collision.

At this point we introduce reduced distribution functions in the following way

$$W_\lambda^{(\nu)}(E;E_1 --- E_\lambda) = \int_\Delta^{E_f} W^{(\nu)}(E;E_1 --- E_\nu)\, dE_{\lambda+1} --- dE_\nu \quad . \tag{3.5}$$

This expresses the probability that in a cascade in which ν recoils are created with energies below E_f, λ will have energies in the specified intervals (E_1,dE_1)---(E_λ,dE_λ). The average number of recoils created can now be written as $\sum_\nu \nu W_0^{(\nu)}(E)$ and the average number created in the interval (E_1,dE_1) as

$$\overline{\nu}(E;E_1)\, dE_1 = \sum_\nu \nu W_1^{(\nu)}(E;E_1)\, dE_1 \quad . \tag{3.6}$$

For this function we can derive an integral equation from (3.4) by integration over dE_2---dE_ν, by multiplication with ν and summation over ν. The result is

$$\begin{aligned}\sum_\nu \nu W_1^{(\nu)}(E;E_1) = &\int_{E_f}^{E-E_f} K(E,T)dT \sum_\nu \sum_{\mu=0}^{\nu} \Big\{\mu W_1^{(\mu)}(E-T;E_1)\, W_0^{(\nu-\mu)}(T) + \\ &\qquad + (\nu-\mu)\, W_0^{(\mu)}(E-T)\, W_1^{(\nu-\mu)}(T;E_1)\Big\} \\ &+ \int_{\Delta}^{E_f} K(E,T)dT \sum_\nu \Big(\delta(T-E_1) W_0^{(\nu-1)}(E-T) + (\nu-1)\, W_1^{(\nu-1)}(E-T;E_1)\Big) + \\ &+ \int_{E-E_f}^{E} K(E,T)dT \sum_\nu \Big(\delta(E-T-E_1)\, W_0^{(\nu-1)}(T) + (\nu-1)\, W_1^{(\nu-1)}(T;E_1)\Big)\end{aligned} \tag{3.7}$$

We can replace $(\nu-\mu)$ by μ' and obtain then in the first term of the right-hand side of (3.7) a double summation over the independent indices μ and μ'. Using the definition (3.6) and the normalization (3.2), Eq. (3.7) can be written as

$$\begin{aligned}\overline{\nu}(E;E_1) = &\int_{\Delta}^{E-E_f} K(E,T)dT\; \overline{\nu}(E-T;E_1) + \int_{E_f}^{E} K(E,T)dT\; \overline{\nu}(T;E_1) \\ &+ \int_{\Delta}^{E_f} K(E,T)dT\,\delta(T-E_1) + \int_{E-E_f}^{E} K(E,T)dT\,\delta(E-T-E_1)\end{aligned} \tag{3.8}$$

It has been shown in Chapter I that for $\gamma = 1$ (equal masses)

$$K(E,T) = \frac{T^{-1-1/s}\, dT}{S(\Delta^{-1/s} - E^{-1/s})} \tag{1.10}$$

normalized to 1, according to $\int_\Delta^E K(E,T)\, dT = 1$. Hence the left-hand side of (3.8) can be written as $\int_\Delta^E K(E,T)\; \overline{\nu}(E;E_1)\, dT$. It is clear that the factor $s(\Delta^{-1/s} - E^{-1/s})$ then cancels out and we are left with the equation

$$(3.9) \quad \int_{\Delta}^{E-E_f} \frac{dT}{T^{1+1/s}} \overline{\nu}(E-T;E_1) - \int_{\Delta}^{E} \frac{dT}{T^{1+1/s}} \overline{\nu}(E;E_1) + \int_{E_f}^{E} \frac{dT}{T^{1+1/s}} \overline{\nu}(T;E_1) + $$
$$+ \frac{1}{E_1^{1+1/s}} + \frac{1}{(E-E_1)^{1+1/s}} = 0$$

which is equivalent to (3.8) .

We rearrange (3.9) as

$$(3.10) \quad \int_{\Delta}^{E-E_f} \frac{dT}{T^{1+1/s}} \left[\overline{\nu}(E-T;E_1) - \overline{\nu}(E;E_1)\right] - \int_{E-E_f}^{E} \frac{dT}{T^{1+1/s}} \overline{\nu}(E;E_1)$$
$$+ \int_{E_f}^{E} \frac{dT}{T^{1+1/s}} \overline{\nu}(T;E_1) + \frac{1}{E_1^{1+1/s}} + \frac{1}{(E-E_1)^{1+1/s}} = 0 \quad .$$

Because of the fact that $E \gg E_f > E_1$ the second and the last terms of (3.10) are very small with respect to the others and will be neglected. For the remaining approximate equation we try the solution $\overline{\nu}(E;E_1) = C(E_f,E_1)\,E$. Substitution yields for C the equation

$$(3.11) \quad -C \frac{(E-E_f)^{1-1/s} - \Delta^{1-1/s}}{1-1/s} + C \frac{E^{1-1/s} - E_f^{1-1/s}}{1-1/s} + \frac{1}{E_1^{1+1/s}} = 0 \quad .$$

In the first term of (3.11), E_f and Δ may be neglected with respect to E and it is easily seen that the asymptotic result ($E \to \infty$) for the collision density then becomes

$$(3.12) \quad \overline{\nu}(E;E_1) = CE = \frac{(1-1/s)\,E}{E_f^{1-1/s}\,E^{1+1/s}}$$

From the results, obtained so far, an important conclusion can be drawn. In the beginning of this chapter we have seen that the average recoil number $\overline{\nu}(E,E_1)\,dE_1$ is composed of two contributions, (1) those which are excited from zero kinetic energy and (2) those which possess kinetic energy above E_f and then are de-excited into the interval (E_1, dE_1) by a single collision. If we had been interested in the first contribution only, we would have taken the probability for de-excitation zero, that is the last term in Eq. (3.4) would not have occurred and occurred and we would have got Eq. (3.8) without the last term on the right-hand side with we have neglected already. From this argument we see the second contribution to the average recoil number is much smaller than the first one.

Another interesting relation can be derived for $\overline{\nu}(E;E_1)$ when use is made of the fact that the sum of the energies of all recoils created in the course of the cascade, if counted in the way that has been described at the beginning of this chapter, must be equal to the initial kinetic energy of the projectile. The normalization relation (3.2) can be rewritten as

$$E\sum_{\nu}\int_0^{E_f} W^{(\nu)}(E;E_1---E_\nu)\,dE_1---dE_\nu = E \quad . \tag{3.13}$$

On the left hand side of (3.13) we replace E by $\sum_{i=1}^{\nu} E_i$, which can be done, because for all combinations of recoil energies where $\sum_i E \neq E$, $W^{(\nu)} = 0$. We find then

$$\sum_{\nu}\int_0^{E_f}\sum_{i=1}^{\nu} E_i W^{(\nu)}(E;E_1---E_\nu)\,dE_1---dE_\nu = E \tag{3.14}$$

which is a symmetrical expression in the E_i and can be replaced by

$$\begin{aligned}\sum_{\nu}\int_0^{E_f}\nu E_1 dE_1\int_0^{E_f} W^{(\nu)}(E;E_1---E_\nu)\,dE_2---dE_\nu &= \\ = \sum_{\nu}\int_0^{E_f}\nu E_1 W^{(\nu)}(E;E_1)dE_1 &= E \quad .\end{aligned} \tag{3.15}$$

Using (3.6) it is now immediately seen that the relation

$$\int_0^{E_f} E_1\overline{\nu}(E;E_1)\,dE_1 = E \qquad \text{is valid.} \tag{3.16}$$

This is a general condition which the collision density must satisfy and it is clear that the asymptotic result (3.12) does indeed satisfy it.

We shall now discuss the phenomenon of a collision cascade from the point of view of probability theory. The cascade can be regarded as an unspecified but great number of collisions ("events") in which one of the two participants in a collision either does or does not come into the interval $(E_1,\Delta E_1)$. This means that it can be conceived of as a series of Bernoulli trials with a variable probability for success in each trial, which is given by the function

$$(3.17) \qquad \left[K(E';E_1) + K(E';E'-E_1)\right] \Delta E_1$$

where E' is the kinetic energy of the moving atom before the collision. The probability that two moving atoms collide is neglected, so in every collision one participant has zero energy before the event.

Consider the explicit form of

$$K(E',E_1) = \frac{E_1^{-1-1/s}}{s(\Delta^{-1/s} - E'^{1-1/s})} \quad .$$

In every collision, which is counted in the cascade $E' > E_f$. If we choose the cut-off energy Δ sufficiently small, so that $\Delta^{-1/s} \gg E_f^{-1/s}$, it is seen that only the second term of (3.23) depends on E'. This means that there is a variable probability for success in each trial only for the second contribution to the recoil number $\bar{\nu}(E;E_1)\Delta E_1$, mentioned previously, which in average is very small compared to the first one. We now make use of a theorem of mathematical statistics[21], which states that the number of successes in a series of Bernouilli-trials with variable chance of success in each trial is approximately distributed according to a Poisson-distribution, if the number of trials is large and the chance of success in each individual trial is small. We can from this draw the conclusion that the number of recoils in the energy interval $(E_1, \Delta E_1)$, $\nu(E;E_1)\Delta E_1$ has a Poisson distribution with mean $\bar{\nu}(E;E_1)dE_1$ as given by (3.14). It follows from the properties of the Poisson-distribution that the variance of the recoil number is given by

$$(3.18) \qquad \overline{(\nu(E;E_1)\Delta E_1 - \bar{\nu}(E;E_1)\Delta E_1)^2} = \bar{\nu}(E;E_1)\Delta E_1$$

from which follows that the relative mean square deviation from the average recoil number is $(\bar{\nu}(E;E_1)\Delta E_1)^{-1}$. It is interesting to compare our calculation with the calculation of $\bar{\nu}(E;E_1)\Delta E_1$, when the atoms interact with each other as hard spheres. This has been dome by Leibfried[20]. The most characteristic property of the hard-sphere interaction is that the energy transfer probability function $K(E',T)dT = dT/E' = K(E';E'-T)$ for equal masses. If we consider again the cascade as a series of Bernoulli-trials, we now see that the probability for success (i.e. the probability that a recoil in a collision will come into $(E_1, \Delta E_1)$ now depends o n l y on ΔE_1 and not on E_1, though it is different in every collision, due to its dependence on E'. From this follows that $\bar{\nu}(E;E_1)$ cannot depend on E_1, and indeed this independence shows in the Leibfried result which is

$$\bar{\nu}(E;E_1) = \frac{2E}{E_f^2} \quad \text{(cf. Fig. 4).}$$

Finally we consider the case that the projectile differs in mass from the target atoms. The only change this causes in the formalism is that the maximum possible energy transfer in a two-particle collision is not the entire kinetic energy E but

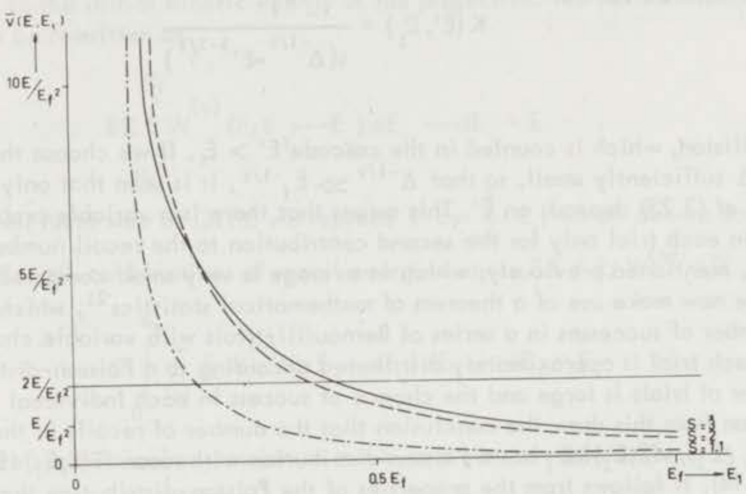

Fig. 4 The behaviour of $\bar{v}(E;E_1)$ as a function of E_1 for three different values of s. The value of s = 1.1 represents the case of a weakly screened interaction. The horizontal straight line is the result for the hard-sphere interaction.

$$T_m = \gamma E = \frac{4\, m_1 m_2}{(m_1+m_2)^2}\; E,$$

where m_1 and m_2 are the masses of projectile and target atom respectively. K (E,T) for this case is given by (1.8). The physical situation is further almost precisely the same as in the case of equal masses. We assume γ to be such that $\gamma E > E_f$. The probability for exciting stationary atoms from zero energy into (E_1, dE_1) is unchanged, but there will be slightly less high-energy recoil atoms in the cascade, due to the fact that the projectile can only transfer a part of its energy in one collision. The amount of recoils which drop into (E_1, dE_1) from an energy above E_f can therefore only be smaller than in the equal mass case. The conclusion is that the average recoil number and its variance are not significantly affected by a change in the mass of the projectile.

It is possible to obtain some information on the direction of motion of recoils, created in a collision cascade. To this end we introduce the function $W^{(\nu)}(E, \vec{n}; E_1, \zeta_1, ---E_\nu, \zeta_\nu)$ representing the probability density function, such that a projectile (with the same mass as the target atoms) has the probability $W^{(\nu)} dE_1 d\zeta_1$--- --$dE_\nu d\zeta_\nu$ of causing a collision cascade in which will be created ν recoils in the energy intervals dE_1--- dE_ν and with directions of motion which make angles with the initial direction of motion $\vec{n}$ of which the cosines lie in the intervals $(\zeta_1, d\zeta_1)$-- --$(\zeta_\nu, d\zeta_\nu)$. The conditions for recoil creation, stated at the beginning of this chapter are again supposed to be valid. This implies that $W^{(\nu)}$ does not depend on the azimuthal angles of the recoil momenta, because every collision of the cascade has azimuthal symmetry and the medium is considered amorphous for all collisions we take into account and is therefore azimuthally symmetric to all recoils with energy $\geqq E_f$. Due to the statistical independence of the two subcascades, started by the participants in the first collision, it is possible to write down an equation analogous to (3.3). But it must be realized that in this case not only the kinetic energies of the participants after the collision are important, but also their directions of motion. We must therefore use the scattering probability function K(E,T) multiplied by angle dependent factors with the angular distribution , as has been done in Chapter I for the differential cross section. The equation for the function $W^{(\nu)}$ then becomes

$$W^{(\nu)}(E,\vec{n};E_1,\zeta_1---E_\nu\zeta_\nu) = \int_\Delta^E K(E,T)dT\,\delta(\vec{n}\vec{n}'-\sqrt{\frac{E-T}{E}})\,\delta(\vec{n}\vec{n}''-\sqrt{T/E})\,\frac{d\Omega' d\Omega''}{2\pi\, 2\pi}\ . \tag{3.19}$$

$$.\sum_{\mu=0}^{\nu}\frac{1}{\binom{\nu}{\mu}}\sum_{P_\alpha} W^{(\mu)}(E-T,\vec{n}';E_{\alpha_1}\zeta'_{\alpha_1}---E_{\alpha_\mu},\zeta'_{\alpha_\mu})W^{(\nu-\mu)}(T,\vec{n}'';E_{\alpha_{\mu+1}},\zeta''_{\alpha_{\mu+1}}---E_{\alpha_\nu},\zeta''_{\alpha_\nu})$$

In this equation ζ' and ζ'' refer to the cosines of the angles which the recoil momenta make with the directions of motion of respectively the projectile and the hit particle after the collision, denoted respectively by $\vec{n}'$ and $\vec{n}''$. Their connections to the ζ are

$$\zeta' = \zeta.\vec{n}\vec{n}' - \sqrt{1-\zeta^2}\,\sqrt{1-\vec{n}\vec{n}'^2}\;\cos(\varphi_2-\varphi_1) \tag{3.20a}$$

$$\zeta'' = \zeta\,\vec{n}\vec{n}'' + \sqrt{1-\zeta^2}\,\sqrt{1-\vec{n}\vec{n}''^{\,2}}\,\cos(\pi-\varphi_2+\varphi_1) \quad . \tag{3.20b}$$

Here φ_2 is the azimuthal angle of the scattering event and φ_1 the azimuthal angle of the recoil momentum. This situation is analogous to the one, described in Chapter II concerning the relation between the angles η' and η (cf. Fig. 1). The vectors $\vec{n}$, $\vec{n}'$ and $\vec{n}''$ lie in one plane, which is the reason that the angle $(\pi-\varphi_2+\varphi_1)$ occurs in Eq. (3.20b).

The next step is the specialization of (3.25) to include the case that one of the participants has an energy below E_f after the first collision. To this end we state that for the case $E < E_f$

$$W^{(\nu)}(E,\vec{n};E_1\zeta_1---E_\nu\zeta_\nu) = \delta_{\nu 1}\prod_{i=1}^{\nu}\delta(E-E_i)\,\delta(\zeta_1-1) \; . \tag{3.21}$$

Like (3.1) this is a direct consequence of the restriction on the recoil number, introduced in the beginning of this chapter, inasmuch that if the initial energy E is smaller than E_f there can only be one recoil in the cascade, namely the projectile itself of which the energy then must be equal to one of the chosen energies E_i, and its direction of motion must coincide with the initial direction of motion $\vec{n}$.
Applying (3.27) to (4.25) we find the equation

$$W^{(\nu)}(E,\vec{n};E_1\zeta_1---E_\nu\zeta_\nu) =$$

$$= \int_{E_f}^{E-E_f} K(E,T)dT\,\delta\Big(\vec{n}\vec{n}'-\sqrt{\tfrac{E-T}{E}}\Big)\delta\big(\vec{n}\vec{n}''-\sqrt{T/E}\big)\frac{d\Omega' d\Omega''}{2\pi\; 2\pi}\sum_{\mu=0}^{\nu}\frac{1}{\binom{\nu}{\mu}}\sum_{P_\alpha}W^{(\mu)}(E-T,\vec{n}';E_{\alpha_1}\zeta'_{\alpha_1}---E_{\alpha_\mu}\zeta'_{\alpha_\mu}) .$$

$$.\,W^{(\nu-\mu)}(T,\vec{n}'';E_{\alpha_{\mu+1}}\zeta''_{\alpha_{\mu+1}}---E_{\alpha_\nu}\zeta''_{\alpha_\nu}) + \int_{\Delta}^{E_f}K(E,T)dT\,\delta\Big(\vec{n}\vec{n}'-\sqrt{\tfrac{E-T}{E}}\Big)\delta\big(\vec{n}\vec{n}''-\sqrt{T/E}\big)\frac{d\Omega' d\Omega''}{2\pi\, 2\pi} .$$

(3.22)

$$.\sum_{\mu=0}^{\nu}\frac{1}{\binom{\nu}{\mu}}\sum_{P_\alpha}\delta_{\mu 1}\prod_{i=1}^{\mu}\delta(T-E_{\alpha_1})\delta(\zeta''_{\alpha_1}-1)\,W^{(\nu-\mu)}(E-T,\vec{n}';E_{\alpha_{\mu+1}}\zeta'_{\alpha_{\mu+1}}---E_{\alpha_\nu}\zeta'_{\alpha_\nu}) \; +$$

$$+\int_{E-E_f}^{E}K(E,T)dT\,\delta\Big(\vec{n}\vec{n}'-\sqrt{\tfrac{E-T}{E}}\Big)\delta\big(\vec{n}\vec{n}''-\sqrt{T/E}\big)\frac{d\Omega' d\Omega''}{2\pi\; 2\pi}\sum_{\mu=0}^{\nu}\frac{1}{\binom{\nu}{\mu}}\sum_{P_\alpha}\delta_{\mu 1}\prod_{i=1}^{\mu}\delta(E-T-E_{\alpha_1})\delta(\zeta'_{\alpha_1}-1)$$

$$.\;W^{(\nu-\mu)}(T,\vec{n}'';E_{\alpha_{\mu+1}}\zeta''_{\alpha_{\mu+1}}---E_{\alpha_\nu}\zeta''_{\alpha_\nu}) \quad .$$

The normalization of the function $W^{(\nu)}$ is as follows

$$\sum_{\nu}\int_{-1}^{1}\int_{\Delta}^{E_f}W^{(\nu)}(E,\vec{n};E_1\zeta_1---E_\nu\zeta_\nu)\,dE_1 d\zeta_1---dE_\nu d\zeta_\nu = 1 \quad . \tag{3.23}$$

We shall now introduce reduced probability functions as before

$$(3.24)\quad W_\lambda^{(\nu)}(E,\vec{n};E_1\zeta_1 --- E_\lambda\zeta_\lambda) = \int_{-1}^{1}\int_{\Delta}^{E_f} W^{(\nu)}(E,\vec{n};E_1\zeta_1 --- E_\nu\zeta_\nu)dE_{\lambda+1}\zeta_{\lambda+1} --- dE_\nu\, d\zeta_\nu$$

As before the average number of recoils created can be written as $\sum_\nu \nu W_0^{(\nu)}(E)$ and the average number in the interval $(E_1,dE_1)(\zeta_1,d\zeta_1)$ as

$$(3.25)\qquad \overline{\nu}(E,\vec{n};E_1,\zeta_1)\,dE_1 d\zeta_1 = \sum_\nu \nu W_1^{(\nu)}(E,\vec{n};E_1,\zeta_1)dE_1\, d\zeta_1$$

For this function, an equation can be derived in the same way as was done for (3.6) from (3.4), i.e. by multiplication with and summation over ν and integration over $E_2\zeta_2 --- E_\nu\zeta_\nu$. The result becomes

$$\overline{\nu}(E,\vec{n};E_1,\zeta_1) = \int_{E_f}^{E-E_f} K(E,T)dT\,\delta(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}})\,\delta(\vec{n}\vec{n}'' - \sqrt{T/E})\,\frac{d\Omega' d\Omega''}{2\pi\, 2\pi}\ \cdot$$

$$(3.26)\qquad \cdot\left[\overline{\nu}(E-T,\vec{n}';E_1,\zeta_1') + \overline{\nu}(T,\vec{n}'';E_1,\zeta_1'')\right] +$$

$$+ \int_{\Delta}^{E_f} K(E,T)dT\,\delta(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}})\,\delta(\vec{n}\vec{n}'' - \sqrt{T/E})\,\frac{d\Omega' d\Omega''}{2\pi\, 2\pi}\Big[\delta(T-E_1)\delta(\zeta_1'-1) + \overline{\nu}(E-T,\vec{n}';E_1\zeta_1')\Big] +$$

$$+ \int_{E-E_f}^{E} K(E,T)dT\,\delta(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}})\,\delta(\vec{n}\vec{n}'' - \sqrt{T/E})\,\frac{d\Omega' d\Omega''}{2\pi\, 2\pi}\Big[\delta(E-T-E_1)\delta(\zeta_1''-1) + \overline{\nu}(T,\vec{n}'';E_1\zeta_1'')\Big]$$

which may be rearranged in the form

$$\overline{\nu}(E,\vec{n},E_1\zeta_1) = \int_{\Delta}^{E-E_f} K(E,T)dT\,\delta(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}})\,\frac{d\Omega'}{2\pi}\,\overline{\nu}(E-T,\vec{n}';E_1,\zeta_1') +$$

$$(3.27)\qquad + \int_{E_f}^{E} K(E,T)dT\,\delta(\vec{n}\vec{n}'' - \sqrt{T/E})\frac{d\Omega''}{2\pi}\,\overline{\nu}(T,\vec{n}'';E_1,\zeta_1'') +$$

$$+ \int_{\Delta}^{E_f} K(E,T)dT\,\delta(\vec{n}\vec{n}'' - \sqrt{T/E})\,\delta(T-E_1)\,\delta(\zeta_1''-1)\,\frac{d\Omega''}{2\pi} +$$

$$+ \int_{E-E_f}^{E} K(E,T)dT\,\delta(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}})\,\delta(E-T-E_1)\,\delta(\zeta_1''-1)\,\frac{d\Omega'}{2\pi}\ .$$

As was done in Chapter II with the range probability density function an expansion into Legendre polynomials is made

$$\overline{\nu}(E;E_1,\zeta_1) = \sum_{\ell=0}^{\infty} (2\ell+1)\,\overline{\nu}_\ell(E;E_1)P_\ell(\zeta_1) \tag{3.28}$$

and the addition theorem for Legendre polynomials (cf. App.B) is used. (The variable $\vec{n}$ is dropped to simplify the notation. Furthermore we use the "closure property" of the Legendre polynomials in the special form

$$\delta(\zeta_1' - 1) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2} P_\ell(\zeta_1') \quad . \tag{3.29}$$

The substitution of (3.28) and (3.29) into (3.27) provides a set of equations for every $\overline{\nu}_\ell$ separately, because the coefficients of the same $P_\ell(\zeta_1)$ on both sides of the equation must be equal. The general equation for $\overline{\nu}_\ell(E;E_1)$ reads

$$\begin{aligned} \overline{\nu}_\ell(E;E_1) = & \int_\Delta^{E-E_f} K(E,T)dT\,\overline{\nu}_\ell(E-T;E_1)P_\ell\left(\sqrt{\frac{E-T}{E}}\right) + \\ & + \int_{E_f}^{E} K(E,T)dT\,\overline{\nu}_\ell(T;E_1)P_\ell(\sqrt{T/E}) + \tfrac{1}{2}\int_{E-E_f}^{E} K(E,T)dT\,\delta(E-T-E_1)\,P_\ell\left(\sqrt{\frac{E-T}{E}}\right) + \\ & + \tfrac{1}{2}\int_\Delta^{E_f} K(E,T)dT\,\delta(T-E_1)\,P_\ell(\sqrt{T/E}) \quad . \end{aligned} \tag{3.30}$$

Consider the case $\ell = 0$. Then (3.30) becomes:

$$\begin{aligned} \overline{\nu}_0(E;E_1) = & \int_\Delta^{E-E_f} K(E,T)dT\,\overline{\nu}_0(E-T;E_1) + \int_{E_f}^{E} K(E,T)dT\,\overline{\nu}_0(T,E_1) \\ & + \tfrac{1}{2}\int_{E-E_f}^{E} K(E,T)dT\,\delta(E-T-E\ ) + \tfrac{1}{2}\int_\Delta^{E_f} K(E,T)dT\,\delta(T-E_1) \end{aligned} \tag{3.31}$$

If this equation is compared with (3.8), it is seen that the only difference is the factor $\frac{1}{2}$ in front of the last two terms. Its solution can be given straight away (with the same degree of accuracy as before, (cf. 3.12)

$$\overline{\nu}_0(E,E_1) = \tfrac{1}{2}\,\frac{(1-1/s)\,E}{E_f^{1-1/s}\,E_1^{1+1/s}} \quad . \tag{3.32}$$

Next we take the case $\ell = 1$. Equation (3.30) then becomes

$$(3.33)\quad \begin{aligned}\overline{\nu}_1(E,E_1) = &\int_{\Delta}^{E-E_f} K(E,T)dT\, \overline{\nu}_1(E-T,E_1)\sqrt{\frac{E-T}{E}} \;+\\ &+\int_{E_f}^{E} K(E,T)dT\, \overline{\nu}_1(T;E_1)\sqrt{T/E} + \tfrac{1}{2}\int_{E-E_f}^{E} K(E,T)dT\,\delta(E-T-E_1)\sqrt{\frac{E-T}{E}} \;+\\ &+\tfrac{1}{2}\int_{\Delta}^{E_f} K(E,T)dT\,\delta(T-E_1)\sqrt{T/E}\quad .\end{aligned}$$

This equation can be solved in the same way as (3.10). Rearrangement of (3.33) gives :

$$(3.34)\quad \begin{aligned}&\int_{\Delta}^{E-E_f} \frac{dT}{T^{1+1/s}}\left[\overline{\nu}_1(E-T,E_1)\sqrt{\frac{E-T}{E}} - \overline{\nu}_1(E,E_1)\right] - \int_{E-E_f}^{E}\frac{dT}{T^{1+1/s}}\,\overline{\nu}_1(E;E_1)\\ &+\int_{E_f}^{E}\frac{dT}{T^{1+1/s}}\,\overline{\nu}_1(T,E_1)\sqrt{T/E} + \tfrac{1}{2}\sqrt{\frac{E_1}{E}}\left(\frac{1}{E_1^{1+1/s}} + \frac{1}{(E-E_1)^{1+1/s}}\right) = 0\ .\end{aligned}$$

The second and last terms of (3.34) can be neglected for the same reason as in the case of (3.10). For the remaining equation we try the solution $\overline{\nu}_1(E,E_1) = C_1(E_f,E_1)\sqrt{E}$. Substitution yields for C_1 the equation

$$(3.35)\quad C_1\int_{\Delta}^{E-E_f}\frac{dT}{T^{1+1/s}}\left[\frac{E-T}{\sqrt{E}} - \sqrt{E}\right] + C_1\int_{E_f}^{E}\frac{dT}{T^{1+1/s}}\,\frac{T}{\sqrt{E}} + \tfrac{1}{2}\sqrt{\frac{E_1}{E}}\,\frac{1}{E_1^{1+1/s}} = 0\ .$$

From (3.35) we find, after we neglect E_f and Δ with respect to E

$$(3.36)\quad C_1 = \tfrac{1}{2}\,\frac{(1-1/s)}{E_f^{1-1/s}\,E_2^{1/2+1/s}}$$

and the solution for $\overline{\nu}_1$ is

$$(3.37)\quad \overline{\nu}_1(E;E_1) = \tfrac{1}{2}\,\frac{(1-1/s)\sqrt{E}}{E_f^{1-1/s}\,E_1^{1/2+1/s}}\quad .$$

So far we found from expansion (3.28) the terms $\overline{\nu}_0$ and $\overline{\nu}_1$. A physical interpretation of these terms will now be given.
If we integrate (3.28) over all values of ζ_1 from -1 to 1, we get by definition the

average number of recoils with energies between E_1 and dE_1, i.e. expression (3.12). This can be restated in the form that (3.28) is multiplied with $P_0(\zeta_1) = 1$ and then integrated. Due to the orthonormality of the P_ℓ all terms of the expansion except $\overline{\nu}_0$ cancel. Hence $2\,\overline{\nu}_0 = \overline{\nu}\,(E;E_1)$ which is immediately seen to agree with (3.32) and (3.12). For $\overline{\nu}_1$ an interpretation can be given also. We multiply (3.28) with $\zeta_1 . \sqrt{2\,mE_1}$ on both sides and then integrate again over $\zeta_1 = P_1(\zeta_1)$. This quantity is equal to the component of the linear momentum of a recoil with kinetic energy between E_1 and $E_1 + dE_1$ in the initial direction of motion of the projectile.The integral

$$\int_{-1}^{1} \sqrt{2mE}_1 \; \zeta_1 \overline{\nu}\,(E,\vec{n};\,E_1\zeta_1)\,d\zeta_1 \tag{3.38}$$

represents therefore the average resulting component of the linear momentum in the direction $\vec{n}$ of all recoils in the energy interval (E_1, dE_1). From the orthogonality relations of the $P_\ell(\zeta_1)$ and (3.28) follows the relation

$$\int_{-1}^{1} \sqrt{2mE}_1 \zeta_1 \; \overline{\nu}\,(E,\vec{n};\,E_1,\zeta_1)d\zeta_1 = 2\;\overline{\nu}_1\;(E,E_1)\;\sqrt{2mE}_1 \tag{3.39}$$

so the term $\overline{\nu}_1(E;E_1)$ is a measure for the resulting momentum of the recoils in (E_1, dE_1).

Finally we shall show that the laws of energy and momentum conservation are satisfied by our expression for $\overline{\nu_0}$ and $\overline{\nu_1}$. We restate the normalization condition (3.29) in the two following ways

$$E\;\sum_\nu \int_0^{E_f}\int_{-1}^{1} W^{(\nu)}(E,\vec{n};\,E_1\zeta_1 --- E_\nu\zeta_\nu)dE_1 d\zeta_1 \;---\; dE_\nu d\zeta_\nu = E \tag{3.40}$$

and

$$\sqrt{2mE}\sum_\nu \int_{\Delta}^{E_f}\int_{-1}^{1} W^{(\nu)}(E,\vec{n};\,E_1\zeta_1 --- E_\nu\zeta_\nu)dE_1 d\zeta_1 --- dE_\nu d\zeta_\nu = \sqrt{2mE}\;. \tag{3.41}$$

We replace (3.40) by

$$\sum_\nu \int_0^{E_f}\int_{-1}^{1} \sum_{i=1}^{\nu} E_i\, W^{(\nu)}(E,\vec{n};\,E_1\zeta_1 --- E_\nu\zeta_\nu)dE_2 d\zeta_2 --- dE_\nu d\zeta_\nu = E\;, \tag{3.42}$$

which is permissible due to energy conservation in the cascade. Because $W^{(\nu)}$ is a symmetric function in the variable pairs $E_i\zeta_i$, (3.40) can be replaced by

$$(3.43)\qquad \sum_{\nu}\int_0^{E_f}\int_{-1}^{1}\nu\, E_1\, dE_1\, d\zeta_1 \int_0^{E_f}\int_{-1}^{1} W^{(\nu)}(E,\vec{n};E_1\zeta_1 --- E\,\zeta\,)dE_2 d\zeta_2 --- dE_\nu d\zeta_\nu =$$

$$= \sum_{\nu}\int_0^{E_f}\int_{-1}^{1}\nu\, E_1\, W_1^{(\nu)}(E,\vec{n};E_1\zeta_1)dE_1\, d\zeta_1 = E\,.$$

Using the definition (3.25) and the expansion (3.28) it is seen that this is equivalent to

$$(3.44)\qquad \int_{\Delta}^{E_f}\int_{-1}^{1} E_1\,\overline{\nu}\,(E,\vec{n};E_1\zeta_1)\,dE_1\, d\zeta_1 = E\,.$$

The law of conservation of momentum demands that the sum of the momenta of all recoils created in the cascade with energies E_f must be equal to the initial momentum of the projectile, which can be stated in the form that the sum of the components of the recoil momenta in the direction $\vec{n}$ must be equal to the initial momentum of the projectile and the sum of the components perpendicular to $\vec{n}$ must be zero. This can be expressed mathematically by $\Sigma_i \sqrt{2mE_i}\,\zeta_i = \sqrt{2mE}$ where the summation is over all recoils in the cascade. This means that (3.41) can be replaced by

$$(3.45)\qquad \sum_{\nu}\int_{\Delta}^{E_f}\int_{-1}^{1}\sum_{i=1}^{\nu}\sqrt{2mE_1}\,\zeta_1 W^{(\nu)}(E,\vec{n};\,E_1\zeta_1 --- E_\nu\zeta_\nu)dE_1 d\zeta_1 --- dE_\nu d\zeta_\nu = \sqrt{2mE}.$$

As $W^{(\nu)}$ is a symmetric function in the sets of variables $E_i\,\zeta_i$ (3.45) can be rewritten as

$$(3.46)\qquad \int_{\Delta}^{E_f}\int_{-1}^{1}\sum_{\nu}\nu\sqrt{2mE_1}\zeta_1 W^{(\nu)}(E,\vec{n};\,E_1\zeta_1 --- E_\nu\zeta_\nu)dE_1 d\zeta_1 --- dE_\nu d\zeta_\nu = \sqrt{2mE}$$

from which follows with the help of (3.30) for the case $\lambda = 1$

$$(3.47)\qquad \int_{\Delta}^{E_f}\int_{-1}^{1}\sqrt{2mE_1}\,\overline{\nu}\,(E,\vec{n};\,E_1\zeta_1)dE_1 d\zeta_1 = \sqrt{2mE}\quad .$$

Eq. (3.47) is the integral of (3.38) over all recoil energies from Δ to E_f and represents therefore the sum of all recoil momentum components in the direction $\vec{n}$. It can now be checked using also (3.48), that our solution (3.32) and (3.37) for $\overline{\nu}_0$ and $\overline{\nu}_1$ satisfy the law of conservation of energy (3.44) and momentum (3.47) respectively, if we take the limit $\Delta \to 0$, which we have done implicitly by neglecting Δ in the solutions of equations (3.31) and (3.35).

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CHAPTER IV

ON THE SPATIAL EXTENSION OF A COLLISION CASCADE

In the preceding section we discussed the average number of low-energy recoils that are created in the cascade of a projectile with kinetic energy E and direction of motion $\vec{n}$. In this section we shall discuss the spatial extension of these recoils, i.e.where they are created with a given energy E_1 in the target material. This is done also with the help of a calculation of moments, which will turn out to be closely analogous to the one carried out for the projectile range.

We begin with the introduction of a probability function for the creation of ν recoils in the energy intervals dE_1 --- dE_ν and in the elements of volume $d\vec{r}_1$ --- $d\vec{r}_\nu$. Here $\vec{r}_1$ --- $\vec{r}$ are co-ordinate vectors with the point of entrance of the projectile as origin. The target is again supposed to be single- or polycrystalline, and again only those recoils are considered which are excited from zero energy into the intervals dE_1 --- dE_ν (E_1; --- $E_\nu \leqq E_f$) or those with energy above E_f which lose so much in a single collision that after it there are in one of those intervals. We denote this probability by

$$(4.1) \qquad W^{(\nu)}(E,\vec{n};E_1,\vec{r}_1 --- E_\nu,\vec{r}_\nu) \cdot dE_1\, d\vec{r}_1 --- dE_\nu\, d\vec{r}_\nu \quad .$$

The projectile is supposed to be of the same species as the target material.

For the case $E < E_f$ we have, due to the above mentioned restriction the relation

$$(4.2) \qquad W^{(\nu)}(E,\vec{n};E_1\vec{r}_1 --- E_\nu\vec{r}_\nu) = \delta_{\nu 1} \prod_{i=1}^{\nu} \delta(E-E_i)\delta(\vec{r}_i) \quad .$$

This means that if the projectile has an energy below E_f, the only recoil in the cascade is the projectile itself which is created at the point of entrance.

The function $W^{(\nu)}$ is normalized according to

$$(4.3) \qquad \sum_{\gamma=0}^{\infty} \int_0^{E_f} \int_{\vec{r}_1 \ldots \vec{r}_\nu} W^{(\nu)}(E,\vec{n};E_1,\vec{r}_1 --- E_\nu\vec{r}_\nu) dE_1\, d\vec{r}_1 --- dE_\nu\, d\vec{r}_\nu = 1.$$

It may be remarked here that $W^{(\nu)}$ is symmetric in the pairs of variables $E_i, \vec{r}_i$. Integration of $W^{(\nu)}$ over coordinates $\vec{r}_1$---$\vec{r}_\nu$ yields the tensity function for recoil energies of Chapter III. We shall now derive the fundamental equation for this function.

We suppose that the projectile, after its entrance into the target moves over a small distance $\Delta\vec{r}$. The probability for a collision with a specified energy transfer and a specified deflection in the direction of motion is then given by $N\,|\Delta\vec{r}\,|\,d\sigma'$, after which both participants in the collision begin statistically independent subcascades. There is also the probability $(1 - N|\Delta\vec{r}|\int d\sigma')$ that the projectile will suffer no collision in the distance $\Delta\vec{r}$.

The balance equation for the probability $W^{(\nu)}$ now reads as follows

$$W^{(\nu)}(E,\vec{n};E_1\vec{r}_i ---E_\nu\vec{r}_\nu) = N|\Delta\vec{r}| \int_{T=E_f}^{T=E-E_f} d\sigma' \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} W^{(\nu)}(E-T\ \vec{n}';$$

$$E_{\alpha_1},\vec{r}_{\alpha_1}-\Delta\vec{r} --- E_{\alpha_\mu}\vec{r}_{\alpha_\mu}-\Delta\vec{r}) \,.\, W^{(\nu-\mu)}(T,\vec{n}'';E_{\alpha_{\mu+1}},\vec{r}_{\alpha_{\mu+1}}-\Delta\vec{r} --- E_{\alpha_\nu}\vec{r}_{\alpha_\nu}-\Delta\vec{r}) +$$

(4.4)

$$+\ N|\Delta\vec{r}| \int_{T=E-E_f}^{T=E} d\sigma' \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} \delta_{\mu 1} \prod_{i=1} \delta(E-T-E_{\alpha_i})\delta(\vec{r}_{\alpha_i}-\Delta\vec{r}) \,.\, W^{(\nu-\mu)}(T,\vec{n}'';$$

$$E_{\alpha_{\mu+1}},\vec{r}_{\alpha_{\mu+1}}-\Delta\vec{r}, --- E_{\alpha_\nu}\vec{r}_{\alpha_\nu}-\Delta\vec{r})$$

$$+\ N|\Delta\vec{r}| \int_{T=\Delta}^{T=E_f} d\sigma' \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} \delta_{\mu 1} \prod_{i=1} \delta(T-E_{\alpha_i})\delta(\vec{r}_{\alpha_i}-\Delta\vec{r})\, W^{(\nu-\mu)}(E-T,\vec{n}';$$

$$E_{\alpha_{\mu+1}},\vec{r}_{\alpha_{\mu+1}}-\Delta\vec{r} --- E_{\alpha_\nu},\vec{r}_{\alpha_\nu}-\Delta\vec{r})$$

$$+\ (1-N|\Delta\vec{r}|\int_{\Delta}^{E} d\sigma')\, W^{(\nu)}(E,\vec{n};E_1,\vec{r}_1-\Delta\vec{r} --- E_\nu,\vec{r}_\nu-\Delta\vec{r})$$

At this point we introduce reduced probability functions

$$(4.5)\quad W_\lambda^{(\nu)}(E,\vec{n};E_1,\vec{r}_i --- E_\lambda,\vec{r}_\lambda) = \int_0^{E_f}\int_{\substack{r_i\\ i=1--\lambda}} W^{(\nu)}(E,\vec{n};E_1\vec{r}_i --- E_\nu\vec{r}_\nu)\, dE_{\lambda+1}\, d\vec{r}_{\lambda+1} --- dE_\nu dr_\nu$$

such that $W^{(\nu)} dE_1 d\vec{r}_1 --- dE_\lambda d\vec{r}_\lambda$ denotes the probability that in the cascade of ν recoils with energies between 0 and E_f there will be λ in the energy intervals $(E_1, dE_1) --- (E_\lambda, dE_\lambda)$ and the elements of volume $d\vec{r}_1 --- d\vec{r}_\lambda$. Let us define of probability density function $W(E,\vec{n}/E_1\vec{r}_1)$ by

$$(4.6)\quad \overline{W}(E,\vec{n};E_1,\vec{r}_1) = \sum_\nu \nu W_1^{(\nu)}(E,\vec{n};E_1,\vec{r}_1)\Big/\bar{\nu}(E,E\ ) = \frac{W(E,\vec{n};E_1,\vec{r}_1)}{\bar{\nu}(E,E_1)}$$

where $\nu(E, E_1)$ is given by (3.6).

One easily verifies that $W(E,n;E,\vec{r})$ is normalized in such a way that $\int \overline{W} d\vec{r}_1 = 1$. It can be interpreted as the probability of finding a recoil in $dE_1 d\vec{r}_1$ when multiplied with $dE_1 dr_1$.

By integration over $E_2, \vec{r}_2 --- E_\nu, \vec{r}_\nu$, multiplication with and summation over ν, the equation for the recoil density can be derived from (4.4.). The result is

$$\sum_\nu \nu W_1^{(\nu)}(E,\vec{n};E_1,\vec{r}_1) =$$

(4.7)
$$\begin{aligned}
&= N|\Delta\vec{r}| \int_{T=E_f}^{T=E-E_f} d\sigma' \sum_{\mu,\mu'} (\mu+\mu') \frac{\mu}{(\mu+\mu')} W_1^{(\mu)}(E-T,\vec{n}';E_1,\vec{r}_1-\Delta\vec{r})\, W_0^{(\mu')}(T) + \\
&+ \frac{\mu'}{(\mu+\mu')} W_0^{(\mu)}(E-T)\, W_1^{(\mu')}(T,\vec{n}'';E_1,\vec{r}_1-\Delta\vec{r}) \quad + \\
&+ N|\Delta\vec{r}| \int_{T=E-E_f}^{T=E} d\sigma' \sum_{\mu,\mu'} (\mu+\mu')\Big[\frac{\delta_{\mu 1}\mu}{(\mu+\mu')} \delta(E-T-E_1)\delta(\vec{r}_1-\Delta\vec{r})\, W_0^{(\mu')}(T) + \\
&+ \frac{\mu'}{(\mu+\mu')} W_1^{(\mu')}(T,\vec{n}'';E_1,\vec{r}-\Delta\vec{r})\Big] + \\
&+ N|\Delta\vec{r}| \int_{T=\Delta}^{T=E_f} d\sigma' \sum_{\mu,\mu'} (\mu+\mu')\Big[\frac{\delta_{\mu 1}\mu}{(\mu+\mu')} \delta(T-E_1)\delta(\vec{r}_1-\Delta\vec{r})\, W_0^{(\mu')}(E-T) + \\
&+ \frac{\mu'}{(\mu+\mu')} W_1^{(\mu')}(E-T,\vec{n}';E_1,\vec{r}_1-\Delta\vec{r})\Big] + (1-N|\Delta\vec{r}|\int^{E} d\sigma') \sum_\nu \nu W_1^{(\nu)}(E,\vec{n};E_1,\vec{r}_1-\Delta\vec{r})
\end{aligned}$$

This equation can with the help of (4.6) be rearranged to the form

(4.8)
$$\begin{aligned}
&\frac{W(E,\vec{n};E_1,\vec{r}_1) - W(E,\vec{n};E_1,\vec{r}_1-\Delta\vec{r})}{|\Delta\vec{r}|} = \\
&= N \int_{T=\Delta}^{T=E-E_f} d\sigma' W(E-T,\vec{n}';E_1,\vec{r}_1-\Delta\vec{r}) + N \int_{T=E_f}^{T=E} d\sigma' W(T,\vec{n}'';E_1,\vec{r}_1-\Delta\vec{r}) - \\
&- N\int_{T=\Delta}^{T=E} d\sigma' W(E,\vec{n};E_1,\vec{r}_1-\Delta\vec{r}) + N\int_{T=\Delta}^{T=E_f} d\sigma' \delta(T-E_1)\delta(\vec{r}_1-\Delta\vec{r}) + \\
&+ N \int_{T=E-E_f}^{T=E} d\sigma' \delta(E-T-E_1)\delta(\vec{r}_1-\Delta\vec{r}) \quad .
\end{aligned}$$

At this point the index 1 from $\vec{r}_1$ will be dropped. Taking the limit $|\Delta\vec{r}| \to 0$ and using the explicit expression for $d\sigma'$, given in Chapter 1, the following equation is obtained

$$\eta \frac{\partial W}{\partial r} + \frac{1+\eta^2}{r} \frac{\partial W}{\partial \eta} = N \frac{\pi}{s} \left\{ \frac{b^2}{4} a^{2s-2} \gamma_s^2 k_s^2 E \right\}^{1/s} \cdot$$

$$(4.9) \quad \cdot \left[\int_{\Delta}^{E-E_f} \frac{dT}{T^{1+1/s}} W(E-T, \eta', r; E_1) \delta\left(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}}\right) \frac{d\Omega'}{2\pi} + \right.$$

$$+ \int_{E_f}^{E} \frac{dT}{T^{1+1/s}} W(T, \eta'', r; E_1) \delta(\vec{n}\vec{n}'' - \sqrt{T/E}) \frac{d\Omega''}{2\pi} -$$

$$- \int_{\Delta}^{E} \frac{dT}{T^{1+1/s}} W(E, \eta, r; E_1) + \frac{\delta(r)}{4\pi r^2} \int^{E_f} \frac{dT}{T^{1+1/s}} \delta(T-E_1) \delta(\vec{n}\vec{n}'' - \sqrt{T/E}) \frac{d\Omega''}{2\pi}$$

$$\left. + \frac{\delta(r)}{4\pi r^2} \int_{E-E_f}^{E} \frac{dT}{T^{1+1/s}} \delta(E-T-E) \delta\left(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}}\right) \frac{d\Omega'}{2\pi} \right]$$

We have made use of the fact that, due to the amorphous nature of the target material the function $W(E, \vec{n}; \vec{r}; E_1)$ depends only on the initial energy E, the recoil energy E_1, the scalar distance from the origin $r = |\vec{r}|$ and the quantity $\eta = (\vec{r}.\vec{n})/r$, which is the cosine of the angle between the initial direction of notion $\vec{n}$ and the radius vector $\vec{r}$. The angles η' and η'' are given by

$$\eta' = \frac{(\vec{r}.\vec{n}')}{r} \quad \text{and} \quad \eta'' = \frac{(\vec{r}.\vec{n}'')}{r} \quad .$$

Also as in Chapter II we shall suppose that $W(E, \eta, r; E_1)$ is an analytic function of E, which enables us to take the limit $\Delta \to 0$. The integrals, occurring in the equations which follow will then be convergent.

Again (cf. Chapter II) we transform to Lindhard's reduced units for distances and energies (2.14), which changes (4.9) into

$$\eta \frac{\partial W}{\partial \rho} + \frac{1-\eta^2}{\rho} \frac{\partial W}{\partial \eta} = \frac{1}{s} \left(\frac{\gamma_s k_s}{2\varepsilon} \right)^{2/s} \varepsilon^{1/s} \left[\int_0^{\varepsilon-\varepsilon_f} \frac{d\tau}{\tau^{1+1/s}} W(\varepsilon-\tau, \eta', \rho; \varepsilon_1) \delta' \frac{d\Omega'}{2\pi} - \right.$$

$$(4.10) \quad - \int_0^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} W(\varepsilon, \eta, \rho; \varepsilon_1) + \int_{\varepsilon_f}^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} W(\tau, \eta'', \rho; \varepsilon_1) \delta'' \frac{d\Omega''}{2\pi} +$$

$$\left. + \frac{\delta(\rho)}{4\pi\rho^2} \int_0^{\varepsilon_f} \frac{d\tau}{\tau^{1+1/s}} \delta(\tau-\varepsilon_1) \delta'' \frac{d\Omega''}{2\pi} + \frac{\delta(\rho)}{4\pi\rho^2} \int_{\varepsilon-\varepsilon_f}^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} \delta(\varepsilon-\tau-\varepsilon_1) \delta' \frac{d\Omega'}{2\pi} \right]$$

$$M_{\ell}^{n}(\varepsilon;\varepsilon_1) = 4\pi \int W_{\ell}(\varepsilon,\rho;\varepsilon_1)\rho^{n+2}\, d\rho$$

Here δ' and δ'' stand for $\delta\left(nn' - \sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\right)$ and $\delta\left(nn'' - \sqrt{\tau/\varepsilon}\right)$.

The integration over the azimuthal angle, contained in $d\Omega'$ and $d\Omega''$ is again over the azimuthal of the scattering event φ_2 as distinct from the azimuthal co-ordinate φ_1 of the chosen element of volume $d\vec{r}$. Therefore, the relation (2.5) is again valid as is an analogous one for η''.

In order to solve (4.10) we apply the same procedure as in Chapter II, i.e. the function $W(\varepsilon,\rho,\eta;\varepsilon_1)$ is expanded in a series of Legendre polynomials as follows

$$W(\varepsilon,\eta,\rho;\varepsilon_1)\rho^2\, d\rho\, d\eta\, d\varphi_1 = \sum_{\ell}(2\ell+1)W_{\ell}(\varepsilon,\rho;\varepsilon_1)\,P_{\ell}(\eta)\rho^2\, d\rho\, d\eta\, d\varphi_1 \tag{4.11}$$

Here $\rho^2 d\rho d\eta d\varphi_1$ is the volume element dr, expressed in reduced polar co-ordinates.

Substitution of (4.11) into (4.10) gives a recursion relation between the different W_{ℓ} by equating the coefficient of the same $P_{\ell}(\eta)$ on both sides

$$\begin{aligned}
&(\ell+1)\frac{\partial W_{\ell+1}}{\partial\rho} + \ell\frac{\partial W_{\ell-1}}{\partial\rho} + (\ell+1)(\ell+2)\frac{W_{\ell+1}}{\rho} - \ell(\ell-1)\frac{W_{\ell-1}}{\rho} = \\
&= \frac{1}{s}\left(\frac{\gamma_s k_s}{2\,\varepsilon}\right)^{2/s}\varepsilon^{1/s}\left[\int_{\delta}^{\varepsilon-\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}(2\ell+1)W_{\ell}(\varepsilon-\tau,\rho;\varepsilon_1)\,P_{\ell}\left(\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\right) - \right. \\
&\quad - \int_{\delta}^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}(2\ell+1)W_{\ell}(\varepsilon,\rho;\varepsilon_1) + \int_{\varepsilon_f}^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}(2\ell+1)W_{\ell}(\tau;\rho,\varepsilon_1)P_{\ell}\left(\sqrt{\tau/\varepsilon}\right) + \\
&\quad + \delta_{\ell 0}\frac{\delta(\rho)}{4\pi\rho^2}\int_{\delta}^{\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}\,\delta(\tau-\varepsilon_1) + \delta_{\ell 0}\frac{\delta(\rho)}{4\pi\rho^2}\int_{\varepsilon-\varepsilon_f}^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}\,\delta(\varepsilon-\tau-\varepsilon_1)
\end{aligned} \tag{4.12}$$

The derivation of (4.12) proceeds in precisely the same way as the derivation of (2.8) and (2.7) (cf. Appendix B). The factor $\delta_{\ell 0}$ is introduced in the last two terms of the right-hand side of (4.12) because these terms are independent of η.

Again as in the case of the ranges we define spatial moments, this time of the recoil density

$$M_{\ell}^{n}(\varepsilon;\varepsilon_1) = 4\pi \int_0^{\infty} W_{\ell}(\varepsilon,\rho;\varepsilon_1)\rho^{n+2}\, d\rho \tag{4.13}$$

The recursion relation for these moments can be derived by multiplication of (4.12) with $4\pi\rho^{n+2}$ and integration over ρ

$$(\ell+1)(\ell-n)M^{n-1}_{\ell+1}(\varepsilon;\varepsilon_1) - \ell(\ell+n+1)M^{n-1}_{\ell-1}(\varepsilon;\varepsilon_1) =$$

$$(4.14)\quad = \frac{(2\ell+1)}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}\varepsilon^{1/s}\left[\int_\delta^{\varepsilon-\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}M^n_\ell(\varepsilon-\tau;\varepsilon_1)P_\ell\left(\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}\right) - \right.$$

$$-\int_\delta^\varepsilon \frac{d\tau}{\tau^{1+1/s}}M^n_\ell(\varepsilon;\varepsilon_1) + \int_{\varepsilon_f}^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}M^n_\ell(\tau;\varepsilon_1)P_\ell(\sqrt{\tau/\varepsilon}) +$$

$$\left. + \delta_{\ell 0}\delta_{n0}\int_\delta^{\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}\delta(\tau-\varepsilon_1) + \delta_{\ell 0}\delta_{n0}\int_{\varepsilon-\varepsilon_f}^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}}\delta(\varepsilon-\tau-\varepsilon_1)\right]$$

Before proceeding with the calculation of the moments, we shall discuss their physical or rather geometrical interpretation. Consider the lowest order moment $M^0_0(\varepsilon;\varepsilon_1)$. From (4.11) and the orthogonality property of the P_ℓ it follows that

$$(4.15)\quad M^0_0(\varepsilon;\varepsilon_1) = 4\pi\int_0^\infty W_0(\varepsilon,\rho;\varepsilon_1)\rho^2 d\rho = \int_{-1}^{1}\int_0^{2\pi}\int_0^\infty W(\varepsilon,\eta;\rho;\varepsilon_1)\rho^2 d\rho d\eta d\varphi_1$$

The zero'th order moment is, therefore, obtained by integrating the recoil density function over all space. Therefore $M^0_0(\varepsilon;\varepsilon_1)d\varepsilon_1$ must of necessity be equal to the average number of recoils, created in the energy interval $(\varepsilon_1, d\varepsilon_1)$ and hence identical with $\overline{\nu}(E;E_1)dE_1$. At the same time it gives the normalization of the recoil density function $W(\varepsilon;\rho;\varepsilon_1)$, as was shown in the discussion of Eq. (4.6). It is seen that the substitution of $\ell = n = 0$ in (4.14) yields the equation (3.9) for $\overline{\nu}(E;E_1)$, if we transform ε back into E.

Consider next the moment $M^1_1(\varepsilon;\varepsilon_1)$. From (4.11) and (4.13) it is evident that

$$(4.16)\quad M^1_1(\varepsilon;\varepsilon_1) = \int_{-1}^{1}\int_0^{2\pi}\int_0^\infty W(\varepsilon,\rho,\eta;\varepsilon_1)\rho^3 d\rho\eta d\eta d\varphi_1 \quad .$$

We can now interpret the quotient $M^1_1(\varepsilon,\varepsilon_1)/M^0_0(\varepsilon;\varepsilon_1)$ as the average value of the projection of the distances from the origin of the created recoils on the initial direction of motion of the projectile. As in the case of the range, this quantity can be written as $\overline{\rho\eta}$. Next, we take the moment $M^2_0(\varepsilon;\varepsilon_1)$. From (4.11) and (4.13) we find

$$(4.17)\quad M^2_0(\varepsilon;\varepsilon_1) = \int_{-1}^{1}\int_0^{2\pi}\int_0^\infty W(\varepsilon,\rho;\eta;\varepsilon_1)\rho^4 d\rho d\eta d\varphi_1$$

The quotient $M_0^2(\varepsilon;\varepsilon_1)/M_0^0(\varepsilon;\varepsilon_1)$ can now be interpreted as the average of the square of the distance from the origin of the recoils in the energy interval $(\varepsilon_1, d\varepsilon_1)$, produced in the collision cascade, and can be written as $\overline{\rho^2}$. From these examples it will be clear that the geometrical interpretation of the quotient M_ℓ^n/M_0^0 is analogous to the one of the moment p_ℓ^n in the case of the range. The moment $M_1^1(\varepsilon;\varepsilon_1)$ will now be calculated by substitution of $n = \ell = 1$ into (4.14). On the left-hand side we get then $-3M_0^0(\varepsilon;\varepsilon_1)$, which may be identified with

$$-\frac{3(1-1/s)\,\varepsilon}{\varepsilon_f^{1-1/s}\,\varepsilon_1^{1+1/s}}$$

The complete equation can be written as

$$-\frac{(1-1/s)\,\varepsilon}{\varepsilon_f^{1-1/s}\,\varepsilon_1^{1+1/s}} = \frac{1}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s} \varepsilon^{1/s}\left[\int_0^{\varepsilon-\varepsilon_f} \frac{d\tau}{\tau^{1+1/s}} M_1^1(\varepsilon-\tau;\varepsilon_1)\sqrt{\frac{\varepsilon-\tau}{\varepsilon_0}} - \right.$$

$$(4.18)\qquad \left. -\int_0^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} M_1^1(\varepsilon;\varepsilon_1) + \int_{\varepsilon_f}^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} M_1^1(\tau;\varepsilon_1)\sqrt{\tau/\varepsilon}\,\right]$$

To find the solution, we proceed in the same way as in the case of the moments of the range, that is, we introduce in (4.14) the variable of integration $y = \tau/\varepsilon$. It then becomes for $n = \ell = 1$.

$$-\frac{(1-1/s)\,\varepsilon}{\varepsilon_f^{1-1/s}\,\varepsilon_1^{1+1/s}} = \frac{1}{s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}\left[\int_0^{1-\varepsilon_f/\varepsilon} \frac{dy}{y^{1+1/s}} M_1^1(\varepsilon-\tau;\varepsilon_1)(1-y)^{\frac{1}{2}} - \right.$$

$$(4.19)\qquad \left. -\int_0^1 \frac{dy}{y^{1+1/s}} M_1^1(\varepsilon;\varepsilon_1) + \int_{\varepsilon_f/\varepsilon}^1 \frac{dy}{y^{1+1/s}} M_1^1(\tau;\varepsilon_1)\, y^{\frac{1}{2}}\right]$$

Since $\varepsilon_f \ll \varepsilon$ we neglect $\varepsilon_f/\varepsilon$ with respect to 1.
As a solution to (4.19) we try the form (cf. the discussion after eq. (2.22))

$$(4.20)\qquad M_1^1(\varepsilon;\varepsilon_1) = \lambda\varepsilon^{1+2/s}$$

where λ is independent of ε, and obtain by substitution an equation for λ which reads

$$(4.21)\quad -\frac{(1-1/s)}{\varepsilon_f^{1-1/s}\varepsilon_1^{1+1/s}} = \frac{1}{s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\lambda\left\{\int_0^1 \frac{dy}{y^{1+1/s}}\left[(1-y)^{3/2+2/s} - 1\right] + \int_0^1 \frac{dy}{y^{1+1/s}}\, y^{3/2+2/s}\right\}$$

The integrals on the right-hand side are now worked out with the resulting equation for λ

$$(4.22)\quad -\frac{(1-1/s)}{\varepsilon_f^{1-1/s}\,\varepsilon_1^{1+1/s}} = \frac{1}{s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s} \lambda \left\{ s - s(3/2+2/s)\,B\,(1-1/s;\,3/2+2/s) + \frac{1}{3/2+1/s} \right\}$$

It follows from the theory of incomplete B-functions that the error we made by neglecting $\varepsilon_f/\varepsilon$ is of the order $(\varepsilon_f/\varepsilon)^{3/2+1/s}$. We therefore have

$$(4.24)\qquad \lambda = \frac{(1-1/s)\,\varepsilon_f^{1/s-1}\,\varepsilon_1^{-(1+1/s)}}{1/s\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\left[s(3/2+2/s)B(1-1/s;\,3/2+2/s) - s - \frac{1}{3/2+1/s}\right]}$$

The average depth under the surface of the recoils created in the energy interval $(\varepsilon_1, d\varepsilon_1)$ is given by the quotient $M_1^1(\varepsilon;\varepsilon_1)/M_0^0(\varepsilon;\varepsilon_1) = \lambda^*\varepsilon^{2/s}$, with $\lambda^* = \lambda/(1-1/s)\,\varepsilon^{1/s-1}\,\varepsilon_1^{-1/s-1}$.

The same calculation can be carried out for $M_0^2(\varepsilon;\varepsilon_1)$ by substituting $n = 2$ and $\ell = 0$ into (4.14). This gives for M_0^2 the following equation

$$(4.25)\quad \begin{aligned} -2M_1^1(\varepsilon;\varepsilon_1) = 5/s\left(\frac{\gamma_s k_s}{2}\right)^{2/s} \varepsilon^{1/s}\Bigg[&\int_0^{\varepsilon-\varepsilon_f} \frac{d\tau}{\tau^{1+1/s}} M_0^2(\varepsilon-\tau;\varepsilon_1) - \int_0^{\varepsilon}\frac{d\tau}{\tau^{1+1/s}} M_0^2(\varepsilon;\varepsilon_1) \\ &+ \int_{\varepsilon_f}^{\varepsilon} \frac{d\tau}{\tau^{1+1/s}} M_0^2(\tau;\varepsilon_1) \end{aligned}$$

(4.25) can be written in a form, analogous to (4.18). The solution is found by again introducing the integration variable $y = \tau/\varepsilon$, and assuming the form $M_0^2(\varepsilon;\varepsilon\ ) = \varkappa\,\varepsilon^{1+4/s}$. This gives for $\varkappa$ the equation

$$(4.26)\quad -2\lambda = 5/s\left(\frac{\gamma_s k_s}{2}\right) \varkappa\left[\int_0^{1-} \frac{dy}{y^{1+1/s}}\left[(1-y)^{1+1/s} - 1\right] + \int_0^1 \frac{dy}{y^{1+1/s}}\, y^{1+1/s}\right]$$

We have neglected again $\varepsilon_f/\varepsilon$ with respect to 1 and after carrying out the integrations we find

$$(4.27)\quad -2\lambda = 5/s\left(\frac{\gamma_s}{2}\right)^{2/s} \varkappa\left[s - s(1+4/s)\,B\,(1-1/s;\,4/s+1) + \frac{1}{3/s+1}\right]$$

from which $\varkappa$ may be determined to be

$$\varkappa = \frac{2\lambda}{5/2\left(\frac{\gamma}{2}\right)^{2/s}\left[(s+4)\,B\,(r\ 1/s;\ 4/s+1) - s - \frac{1}{3/s+1}\right]} \tag{4.28}$$

to an accuracy of the order $(\varepsilon_f/\varepsilon)^{3s+1}$. The mean square of the distance from the origin of the recoils, created in the interval $(\varepsilon_1, d\varepsilon_1)$ is given by $M_0^2(\varepsilon;\varepsilon_1)/M_0^0(\varepsilon;\varepsilon_1) = \varkappa^*\,\varepsilon^{4/s}$, where

$$\varkappa^* = \frac{2\lambda^*}{5/2\left(\frac{\gamma}{2}\right)^{2/s}\left[(s+4)\,B\,(1-1/s;4/s+1) - s - \frac{1}{3/s+1}\right]}$$

The analogy with the calculation of the range moments $p_\ell^n(\varepsilon)$ can be observed from these two examples. All $M_\ell^n(\varepsilon;\varepsilon_1)$ with $n+\ell$ even and $n \geqq \ell$ can be calculated successively from the recurrence relation (4.14) by putting $M_\ell^n(\varepsilon;\varepsilon_1) \sim \varepsilon^{1+2n/s}$. We now want to generalize this treatment for the case that the projectile differs from the target material. We shall first consider the case that the maximum energy transfer between the projectile and a target particle in a single collision $T_m = \gamma E < E - E_f$, which means that the projectile can never lose so much energy in its first collision that it retains less than E_f. In that case we introduce for the projectile the probability function $V^{(\nu)}(E,\vec{n};E_1,\vec{r}_1 \text{ --- } E_\nu,\vec{r}_\nu)$, which has the same meaning as (4.1). In its first collision after entrance into the target material it hits of course a target atom which is of the same species as all other target atoms. Furthermore, the normalization of $V^{(\nu)}$ is the same as that of $W^{(\nu)}$ (cf. (4.3)) and it is also symmetric in the pairs of variables E_i, r_i. From these facts, the balance equation for $V^{(\nu)}$, analogous to (4.4) can be shown to be

$$V^{(\nu)}(E,\vec{n};E_1,\vec{r}_1 \text{ --- } E_\nu \vec{r}_\nu) =$$

$$= N|\Delta\vec{r}| \int_{T=E_f}^{T=\gamma E} d\sigma \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} V^{(\mu)}(E-T,\vec{n}\,';E_{\alpha_1}\vec{r}_{\alpha_1} - \Delta\vec{r}\,E_{\alpha_\nu}\vec{r}_{\alpha_\nu} - \Delta\vec{r}) \,.$$

$$\cdot\, W^{(\nu-\mu)}(T,\vec{n}\,'';E_{\alpha_{\mu+1}}\vec{r}_{\alpha_{\mu+1}} - \Delta\vec{r};E_{\alpha_\nu},\vec{r}_{\alpha_\nu} - \Delta\vec{r}) + N|\Delta\vec{r}| \int_{T=\Delta} d\sigma' \sum_{\mu=0}^{\nu} \frac{1}{\binom{\nu}{\mu}} \sum_{P_\alpha} \delta_{\mu 1} \,\cdot \tag{4.29}$$

$$\cdot \prod_{i=1}^{\mu} \delta(T-E_{\alpha_i})\,\delta(\vec{r}_{\alpha_i} - \Delta\vec{r})\,V^{(\nu-\mu)}(E-T,\vec{n}\,';E_{\alpha_{\mu+1}}\vec{r}_{\alpha_{\mu+1}} - \Delta\vec{r}\,E_{\alpha_\nu}\vec{r}_{\alpha_\nu} - \Delta\vec{r}) \;+$$

$$+\;(1 - N|\Delta\vec{r}| \int_{T=\Delta}^{T=E} d\sigma')\,V^{(\nu)}(E,\vec{n};E_i,\vec{r}_i - \Delta\vec{r}, \text{ --- } E_\nu,\vec{r}_\nu - \Delta\vec{r})$$

At this point the reduced distribution functions $V_\lambda^{(\nu)}$, analogous to $W_\lambda^{(\nu)}$ are introduced and the recoil density in the collision cascade, caused by the projectile is defined as

$$V(E,\vec{n};E_1,\vec{r}_1) = \sum_\nu \nu V_1^{(\nu)}(E,\vec{n};E_1,\vec{r}_1) \quad . \tag{4.30}$$

If we integrate (4.29) over $E_2, \vec{r}_2$ ---E_r $\vec{r}_\nu$, multiply with and sum over ν, we find for $V(E,\vec{n};E_1,\vec{r}_1)$ the equation

$$\begin{aligned} V(E,\vec{n};E_1,\vec{r}_1) &= N|\Delta\vec{r}| \int_{T=\Delta}^{T=\gamma E} d\sigma' \, V(E-T,\vec{n}';E_1,\vec{r}_1-\Delta\vec{r}) + \\ &+ N|\Delta\vec{r}| \int_{T=E_f}^{T=\gamma E} d\sigma' \, W(T,\vec{n}'';E_1,\vec{r}_1-\Delta\vec{r}) + N|\Delta\vec{r}| \int_{T=\Delta}^{T=E_f} d\sigma' \, \delta(T-E_1) \, . \, \delta(\vec{r}_1-\Delta\vec{r}) \quad + \\ &+ \left(1-N|\Delta\vec{r}| \int_{T=\Delta}^{T=\gamma E} d\sigma'\right) V(E,\vec{n};E_1,\vec{r}_1-\Delta\vec{r}) \, . \end{aligned} \tag{4.31}$$

(4.31) is rearranged in the same way as (4.7) by bringing the term $V(E,\vec{n};E\ \vec{r}-\Delta\vec{r})$ to the other side and dividing the equation by $|\Delta\vec{r}|$. We then again drop the index 1 from $\vec{r}_1$, introduce the co-ordinates r and η and take the limit $|\Delta\vec{r}| \to 0$. Eq. (4.31) is then reduced to a form corresponding to (4.9), when the explicit form of $d\sigma'$ is introduced

$$\begin{aligned} &\eta \frac{\partial V}{\partial r} + \frac{1-\eta^2}{r} \frac{\partial V}{\partial \eta} = N \frac{\pi}{s} \left\{ \frac{b^2}{4} a^{2s-2} \, k_s^2 \gamma_s^2 T_m \right\}^{1/s} . \\ &\cdot \left[\int_0^{\gamma E} \frac{dT}{T^{1+1/s}} V(E-T,\eta',r;E_1) \delta\left(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}} \frac{m_1+m_2}{2m_1} - \sqrt{\frac{E}{E-T}} \frac{m_1-m_2}{2m_1}\right) \frac{d\Omega'}{2\pi} \right. \\ &- \int_0^{\gamma E} \frac{dT}{T^{1+1/s}} V(E,\eta,r;E_1) + \int_{E_f}^{\gamma E} \frac{dT}{T^{1+1/s}} W(T,\eta'',r;E_1) \delta\left(\vec{n}\vec{n}'' - \frac{m_1+m_2}{2\sqrt{m_1 m_2}} \sqrt{T/E}\right) . \\ &\left. \cdot \frac{d\Omega''}{2\pi} + \frac{\delta(r)}{4\pi r^2} \int_0^{E} \frac{dT}{T^{1+1/s}} \delta(T-E_1) \delta\left(\vec{n}\vec{n}'' - \frac{m_1+m_2}{2\sqrt{m_1 m_2}} \sqrt{T/E}\right) \frac{d\Omega''}{2\pi} \right] \end{aligned} \tag{4.32}$$

Here m_1 and m_2 are the masses of respectively the projectile and the target atom.

We want to transform eq. (4.32) to the reduced units for energies and distances (cf. (2.28)). It must be realized that we now have two sets of reduced units, namely for the case of the interaction between the projectile and a target atom and for the interaction of two target atoms amongst themselves. If we call the first set ε and ρ, the second set can be written as $\varepsilon'=\alpha\varepsilon$ and $\rho'=\beta\rho$, where α and β are constants which can easily be calculated from the definition (2.28). This yields the following reduced equation

$$\eta\frac{\partial V}{\partial\rho}+\frac{1-\eta^2}{\rho}\frac{\partial V}{\partial\eta}=\frac{1}{\gamma_s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}(\gamma\varepsilon)^{1/s}\;.$$

$$\cdot\left[\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}V(\varepsilon-\tau,\eta'',\rho;\varepsilon_1)\delta\left(\vec{n}\vec{n}'-\frac{m_1+m_2}{2m_1}\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}-\frac{m_1-m_2}{2m}\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\right)\frac{d\Omega'}{2\pi}-\right.$$

$$(4.33)\quad -\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}V(\varepsilon,\eta,\rho;\varepsilon_1)+\alpha^{-1/s}\int_{\varepsilon_f}^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}W(\alpha\tau,\eta'',\beta\rho;\varepsilon_1)\delta\left(\vec{n}\vec{n}''-\frac{m_1+m_2}{2\sqrt{m_1m_2}}\sqrt{\tau/\varepsilon}\right)\frac{d\Omega}{2\pi}+$$

$$\left.+\frac{\delta(\beta\rho)}{4\pi(\beta\rho)^2}\alpha^{-1/s}\int_0^{\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}\delta(\alpha\tau-\alpha\varepsilon)\,\delta\left(\vec{n}\vec{n}''-\frac{m_1+m_2}{2\sqrt{m_1m_2}}\sqrt{\tau/\varepsilon}\right)\frac{d\Omega''}{2\pi}\right]$$

We can again expand the functions V and W into Legendre polynomials of η and then introduce spatial moments, which are defined by

$$(4.34^a)\quad N^n_\ell(\varepsilon;\varepsilon_1)=4\pi\int_0^\infty V_\ell(\varepsilon,\rho;\varepsilon_1)\rho^{m+2}d\rho\quad\text{and}$$

$$(4.34^b)\quad M^n_\ell(\varepsilon;\varepsilon_1)=4\pi\int_0^\infty W_\ell(\alpha\varepsilon;\beta\rho;\varepsilon_1)(\beta\rho)^{n+2}d(\beta\rho)\;.$$

This results in the moment equation

$$(\ell+1)(\ell-n)N^{n-1}_{\ell+1}(\varepsilon;\varepsilon_1)-\ell(\ell+n+1)N^{n-1}_{\ell-1}(\varepsilon;\varepsilon_1)=\frac{(2\ell+1)}{\gamma_s}\left(\frac{\gamma_s k_s}{2\varepsilon}\right)^{2/s}(\gamma\varepsilon)^{1/s}\;.$$

$$\cdot\left[\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}N^n_\ell(\varepsilon-\tau;\varepsilon_1)\,.\,P_\ell\left(\frac{m_1+m_2}{2m_1}\sqrt{\frac{\varepsilon-\tau}{\varepsilon}}+\frac{m_1-m_2}{2m_1}\sqrt{\frac{\varepsilon}{\varepsilon-\tau}}\right)-\right.$$

$$-\int_0^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}N^n_\ell(\varepsilon;\varepsilon_1)+\alpha^{-1/s}\beta^{-(n+3)}\int_{\varepsilon_f}^{\gamma\varepsilon}\frac{d\tau}{\tau^{1+1/s}}M^n_\ell(\tau;\varepsilon_1)P_\ell\left(\frac{m_1+m_2}{2\sqrt{m_1m_2}}\sqrt{\tau/\varepsilon}\right)+$$

$$\left.+\delta_{\ell 0}\delta_{n0}\,\alpha^{-1/s}\int_0^{\varepsilon_f}\frac{d\tau}{\tau^{1+1/s}}\delta(\alpha\tau-\alpha\varepsilon)\right.$$

Because the moments $M^n_\ell(\varepsilon;\varepsilon_1)$ have been found before, the $N^n_\ell(\varepsilon;\varepsilon_1)$ can be calculated from this recursion relation. The geometrical interpretation of the $N^n_\ell(\varepsilon;\varepsilon_1)$ is the same as that of the $M^n_\ell(\varepsilon:\varepsilon_1)$. N^0_0, like M^0_0 is obtained by integrating the recoil density function $V(\varepsilon,\eta,\rho;\varepsilon_1)$ over all space and is, therefore, the average number of

the recoils created. Of course, like in the case of equal masses the average depth of the created recoils is now given by $N_1^1(\varepsilon;\varepsilon_1)/N_0^0(\varepsilon\,\varepsilon_1)$, and the quotients of all higher moments and N_0^0 have the same geometrical meaning as M_ℓ^n/M_0^0.
It has been argued in the preceding chapter that N_0^0 is not influenced by a change in rhe mass of the projectile. It can then be shown that the case $\gamma E > E - E_f$ can be analized as well and yields for the calculable moments the same results.

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CHAPTER V

FURTHER DETAILS ON RANGE AND CASCADE DISTRIBUTIONS AND COMPARISONS WITH EXPERIMENT

In this chapter we shall make comparisons between moments of the range and of the spatial cascade extension and we shall also consider ratios of range and cascade moments amongst themselves[21]. Finally we shall compare some of the theoretical results with experiments. As several authors[22,23] have made calculations on moments of ranges and spatial distributions of radiation damage with the help of a hard-sphere model, it will be useful to compare the results obtained by the use of a power potential for the interatomic interaction in the preceding chapters, with the same quantities, calculated with a hard-sphere model.

It can very easily be proved[3] that the differential cross section for an energy transfer between T and T + dT in a collision between to rigid spheres can be written as

$$d\sigma_{HS} = \sigma_{HS}(E)\,\frac{dT}{T_m} \tag{5.1}$$

where $T_m = \gamma E$ = maximum energy transfer and σ_{HS} is the total cross section, which is dependent on E. We shall determine it in the following way.

Consider the stopping power, i.e. the mean energy loss per unit path length of a projectile with the energy E in target matter. This is defined as

$$S = \frac{1}{N}\,\frac{dE}{dr} = \int_0^{T_m} T\,d\sigma \tag{5.2}$$

and for the power potential cross sections which we used hitherto it is equal to (cf. (1.4))

$$S = \frac{\pi}{s}\left\{\frac{b^2}{4}\,a^{2s-2}\,k_s^2\gamma_s^2\,T_m\right\}^{1/s}\frac{T_m^{\,1-1/s}}{1-1/s} = \frac{C\,\gamma^{1-1/s}}{1-1/s}\,E^{1-2/s} \tag{5.3}$$

where C simply is the factor which remains if we separate the product

$$\frac{\gamma^{1-1/s}\,E^{1-2/s}}{1-1/s}$$

out of the second member of (5.3).

For a hard-sphere cross section the stopping power becomes

$$S_{HS} = \int_0^{T_m} T\sigma_{HS}(E)\,\frac{dT}{T_m} = \tfrac{1}{2}\,\sigma_{HS}(E)\,.\,T_m \tag{5.4}$$

We now define the total hard-sphere cross section $\sigma_{HS}(E)$ by equating (5.3) and (5.4) , from which follows that

$$\sigma_{HS}(E) = \frac{2}{1-1/s}\,C\gamma^{-1/s}\,E^{-2/s} \tag{5.6}$$

The first quantity which we shall consider is the ratio

$$p_1^1(\varepsilon)\,.\,M_0^0(\varepsilon;\varepsilon_1)/M_1^1(\varepsilon;\varepsilon_1)$$

which for normal incidence of the projectile is the ratio between the mean penetration depth $p_1^1(\varepsilon)$ of projectiles with incoming energy ε and the mean depth

$$\frac{M_1^1(\varepsilon;\varepsilon_1)}{M_0^0(\varepsilon;\varepsilon_1)}$$

at which recoils of some energy below ε_f are created. We shall take first the case of equal masses of projectile and target particles. After a simple algebraic calculation, starting from (2.22) and (4.24a) it then turns out that

$$\frac{p_1^1(\varepsilon)\;M_0^0(\varepsilon;\varepsilon_1)}{M_1^1(\varepsilon;\varepsilon_1)} = \frac{3/2 + 2/s}{3/2 + 1/s} = \frac{<x>}{<x_D>} \tag{5.6}$$

where we denote by $<x>$ and $<x_D>$ the mean depth of penetration of the projectiles and of the radiation damage created respectively. This expression is almost a constant for all exponents of interest, because it varies from 1.31 for $s = 1.5$ to 1.14 for $s = 4$. As all realistic interatomic potentials for collisions in the 20 to 50 keV energy range in which we are interested, behave approximately as inverse power potentials with the exponent s in the interval mentioned here, it may be concluded that the ratio $<x>/<x_D>$ will always be close to 1. Of course, it follows from the results of chapters II and IV that it is independent of the projectile energy. So the ratio $<x>/<x_D>$ is in all cases considered above greater than one, which means that for all potentials considered the average penetration depth of the projectile is greater than the average depth of the damage created.

With the help of (2.31) and (4.38) we can calculate $<x>/<x_D>$ as a function of the mass ratio m_2/m_1 of target-atom and projectile masses. The result is given in Fig. 5 and it shows that for not too different masses it remains of the order of 1.

The same comparison can be made for the second-order moments of range and damage extension. In this case attention is focused on the variances of the penetration and damage depth, which are given by the expressions in the moments (Cf. Ch. II).

$$(5.7^a)\qquad \frac{1}{3}p_0^2(\varepsilon)+\frac{2}{3}p_2^2(\varepsilon)-(p_1^1(\varepsilon))^2$$

and for the damage extension the analogous expression

$$(5.7^b)\qquad \frac{\frac{1}{3}M_0^2(\varepsilon;\varepsilon_1)+\frac{2}{3}M_2^2(\varepsilon;\varepsilon_1)}{M_0^0(\varepsilon;\varepsilon_1)}-\left(\frac{M_1^1(\varepsilon;\varepsilon_1)}{M_0^0(\varepsilon;\varepsilon_1)}\right)^2$$

which in our present notation can be denoted by $<\Delta x^2> = <(x-<x>)^2>$ and $<\Delta x_D^2> = <(x_D-<x_D>)^2>$.

(5.7^a and (5.7^b) have been calculated numerically both for the cases of equal and unequal masses of projectile and target atoms. The results will be given numerically for the equal mass case in the tables which follow, and which, of course, are based on the results of chapters II and IV. As a function of the mass ratio they are shown in Fig. 6. These tables contain also some other moments of interest, namely the first-order ones $<x>$ and $<x_D>$ and the mean square of the transverse extention $<y^2>$ and $<y_D^2>$, which expressed in the moments p_ℓ^n and M_ℓ^n/M_0^0 are equal to resp.

$$(5.8^a)\qquad <y^2> = 2/3\,(p_0^2(\varepsilon)-p_2^2(\varepsilon)) \quad \text{and}$$

$$(5.8^b)\qquad <y_D^2> = 2/3\left(\frac{M_0^2(\varepsilon;\varepsilon_1)-M_2^2(\varepsilon;\varepsilon_1)}{M_0^0(\varepsilon;\varepsilon_1)}\right)$$

TABLE (5.1^a)

s	$<x>/(\varepsilon^{2/s}.C_1)$	$\frac{<\Delta x^2>}{<x>^2}$	$\frac{<y^2>}{<x>^2}$
1.5	0.204 (0.258)	0.204 (0.652)	0.145 (0.064)
2	0.369 (0.417)	0.276 (0.611)	0.176 (0.095)
3	0.597 (0.619)	0.341 (0.568)	0.241 (0.159)
4	0.750 (0.750)	0.385 (0.556)	0.308 (0.222)

The factor $C_1 = \frac{1}{s}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}$

TABLE (5.1[b])

s	$\langle x_D \rangle / (\varepsilon^{2/s} . C_1)$	$\langle \Delta x_D^2 \rangle / \langle x_D \rangle^2$	$\langle y_D^2 \rangle / \langle x_D \rangle^2$
1.5	0.156 (0.348)	0.337 (0.489)	0.130 (0.092)
2	0.295 (0.583)	0.380 (0.451)	0.157 (0.132)
3	0.505 (0.905)	0.407 (0.423)	0.220 (0.210)
4	0.656 (1.125)	0.429 (0.429)	0.286 (0.286)

The numbers between brackets in tables (5.1[a]) and (5.1[b]) give the corresponding results for the hard-sphere model as defined in the beginning of this chapter. The following tables give these same rations for the case s = 2 and different values of m_2/m_1.

TABLE (5.2[a])

m_2/m_1	$\frac{\langle x \rangle}{\varepsilon C_1}$	$\frac{\langle \Delta x^2 \rangle}{\langle x \rangle^2}$	$\frac{\langle y^2 \rangle}{\langle x \rangle^2}$
0.1	0.842	0.058	0.018
0.25	0.577	0.125	0.044
0.5	0.453	0.195	0.089
1	0.369	0.275	0.176
2	0.297	0.409	0.343
4	0.229	0.710	0.674
10	0.153	1.684	1.671

TABLE (5.2[b])

m_2/m_1	$\frac{\langle x_D \rangle}{\varepsilon C_1}$	$\frac{\langle \Delta x_D^2 \rangle}{\langle x_D \rangle^2}$	$\frac{\langle y_D^2 \rangle}{\langle x_D \rangle^2}$
0.1	0.692	0.434	0.192
0.25	0.489	0.437	0.181
0.5	0.376	0.386	0.152
1	0.295	0.380	0.157
2	0.241	0.457	0.257
4	0.198	0.623	0.485
10	0.143	0.215	1.153

In these tables it has been assumed that $Z_2/Z_1 = m_2/m_1$.

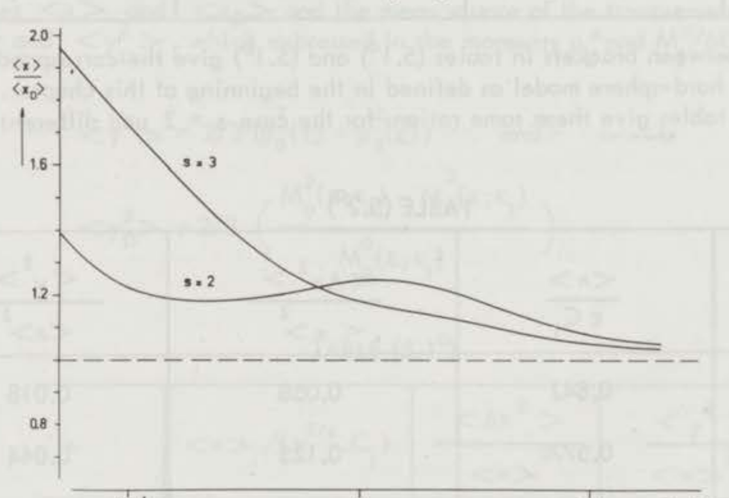

Fig. 5 Ratio of the average penetration depth and average depth of created damage as a function of the mass-ratio m_2/m_1.

From the results collected so far some interesting conclusions can be drawn.

Considering the first-order moments, we see that in all cases $\langle x \rangle > \langle x_D \rangle$ for power scattering, which means that the projectile in the average comes to rest behind the average depth of the cascade. It follows from tables (5.1[a]) and (5.1[b]) that for hard-sphere interactions, at least in the equal mass case, the reverse is true. It has already been mentioned that for power scattering $<x> \approx <x_D>$. As follows from Fig. 5 this is true for $s = 2$ for practically all values of m_2/m_1 and for $s = 3$ for $m_2/m_1 \geqq 0.5$. For extremely light projectiles, $<x>$ and $<x_D>$ become identical, while for extremely heavy projectiles the range becomes considerably greater than the average damage depth.

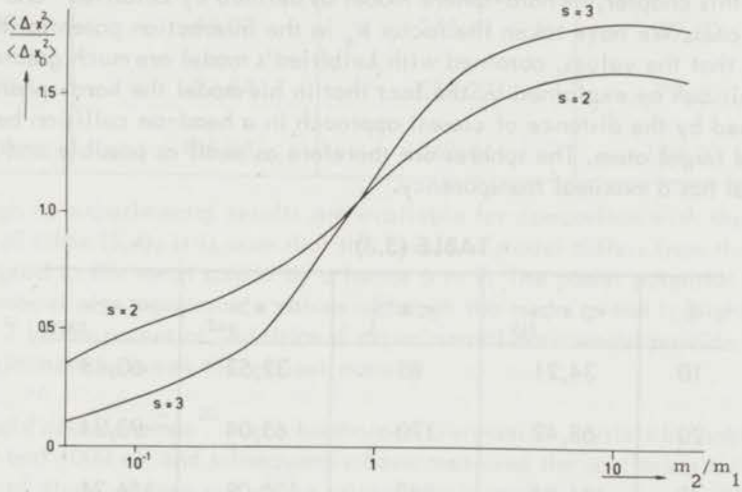

Fig. 6 Ratio of the variances of penetration and damage depth as a function of m_2/m_1.

From tables (5.1^a) and (5.1^b) it follows that for $m_1 = m_2$ $\frac{<\Delta x^2>}{<\Delta x_D^2>} = 1.1 \pm 0.1$ for $1.5 \leqq s \leqq 4$, which means that it will be difficult to distinguish experimentally between range and damage distributions. For hard-sphere scattering we find $<\Delta x^2>/<\Delta x_D^2> = 0.7 \pm 0.1$, which means that the range distribution would be narrower than the damage distribution. It is seen that for $m_1 >> m_2$ the range distribution is much sharper than the damage distribution, while for $m_1 << m_2$ the damage distribution is somewhat sharper than the range distribution.

Finally we mention the transverse extensions. It is found from tables (5.1^a) and (5.1^b) that

$$\frac{<y^2>/<x^2>}{<y_D^2>/<x_D^2>} = 1.11 \pm 0.02 \quad \text{or} \quad \frac{<y^2>}{<y_D^2>} = 1.6 \pm 0.3.$$

It is worthwhile to note that both range and damage distributions are much more elongated for power scattering than for hard-sphere scattering. This has also been found by Oen, Holmes and Robinson [24] in numerical calculations on ranges of energetic atoms (1 to 100 keV) in amorphous solids.

We shall now make some comparisons of theoretical with experimental results. Unfortunately there is not sufficient experimental data to compare with all theoretical quantities, calculated in the preceding chapters.

Domey et al.[18] have measured the mean penetration depth $<x>$ of $^{85}Kr^{+}$-ions into amorphous Al_2O_3. In table (5.3) we give a comparison between values of $<x>$ calculated with the power potential with s = 2, used in Chapter II, the hard-sphere model as defined in this chapter, the hard-sphere model as defined by Leibfried[9] and the experimental ones. We have taken the factor k_s in the interaction potential to be 1. It is observed that the values, obtained with Leibfried's model are much greater than the others. This can be explained by the fact that in his model the hard-sphere radius is defined by the distance of closest approach in a head-on collision between projectile and target atom. The spheres are therefore as small as possible and the target material has a maximal transparency.

TABLE (5.3)

E	$<x>_{HS}$	$<x>_{L}$	$<x>_{s=2}$	$<x>_{exp}$
10	34,21	85	32,52	60,48
20	68,42	170	65,04	93,24
40	136,84	340	130,08	156,24
80	273,68	680	260,16	269,64
160	547,36	1360	520,32	514,08

(All distances are given in Å and the energies in keV.)

It is seen that for energies above 20 keV the Leibfried hard-sphere model overestimates the mean penetration depth by roughly a factor 2. On the other hand the power potential with s = 2 yields very satisfactory values. The hard-sphere model as defined in this chapter gives values which are equally acceptable. This may be explained by the fact that the hard-sphere radius is defined here in such a way as to yield the same stopping power as the s = 2 power potential.

In table (5.4) we compare the values of the mean spread about average for the three potentials.

TABLE (5.4)

E	$\sqrt{<x^2>-<x>^2}_{HS}$	$\sqrt{<x^2>-<x>^2}_{L}$	$\sqrt{<x^2>-<x>^2}_{s=2}$
10	11,58	66,40	9,95
20	23,16	132,81	19,90
40	46,32	265,61	39,80
80	92,64	531,22	79,60
160	185,28	1062,44	159,20

Although no experimental results are available for comparison with the theoretical values of table (5.4), it is seen that the Leibfried model differs from the other two with regard to the mean spread by a factor 6 to 7. The power potential and the hard sphere model give comparable values although the mean spread is slightly lower for the s = 2 power potential. Additional experimental data would provide further means to discriminate between the various models.

McDonald and Haneman[25] have bombarded Germanium crystals by noble gas ions of 500 eV and 1000 eV and subsequently have measured the sputtering ratio i.e. the number of atoms, thrown out of the crystal per incoming ion, due to 200 eV Ar-ions. Onderdelinden[14] has shown that the sputtering ratio of a single crystal is strongly dependent on the accessibility of the open channels of the lattice (Cf. Chapter I). If damage is caused by bombardment many of these channels will be blocked by interstitial atoms and it follows from Onderdelinden's work that the sputtering ratio increases. This is what McDonald and Haneman indeed observe, when they measure the change in the sputtering ratio as the atomic layers in which the damage is introduced are successively eroded away. In this way the depth over which the sputtering ratio is influenced, can be measured.

There is an uncertainty whether this change is caused by damage of the crystal lattice, or by non channeling projectiles which are stopped in the lattice after they have lost their initial kinetic energy. If the non channeling projectiles do not enter an open direction, they interact with the lattice as if it were amorphous, and hence the theory of Chapter II may be applied to them. If they come to rest, after having lost their energy, they also can block open channels, and therefore, can have the same effect upon the sputtering ratio as interstitial atoms. We shall compare in Table (5.5) the experimentally measured thicknesses of the layers over which the sputtering ratio is changed with theoretical values of penetration depth of projectiles and damage extensions. For these we take the expressions

$$<x> + <\Delta x^2>^{\frac{1}{2}} \quad \text{and} \quad <x_D> + <\Delta x_D{}^2>^{\frac{1}{2}} ,$$

calculated for s = 2, which are the sums of the average depth plus the root mean square deviation for the energies of 500 and 1000 eV with which the bombardment were performed.

TABLE (5.5)

energy	500 eV				1000 eV			
projectile	He	Ne	Ar	Kr	He	Ne	Ar	Kr
$<x> + <x^2>^{\frac{1}{2}}$	120	32	21	14	230	51	34	23
$<x_D> + <x_D^2>^{\frac{1}{2}}$	100	27	18	13	200	42	29	20
Observed depth		26	16	13	16.5	40	35	30

All distances have been expressed in Å. It is seen that both the theoretical range and damage distributions are consistent with experimental results. Only the bombardment with 100 eV He-ions produces results which cannot be explained by theory. This may be due to the fact that He-ions of so low an energy will not produce a significant amount of damage, due to the low stopping power. Also Schiøtt[26] and Kistemaker c.s.[28] pointed out that for the case $Z_1 \ll Z_2$ it is not allowed to neglect the explicit contribution to the stopping of the electron gas of the target matter, which we have done throughout this work.

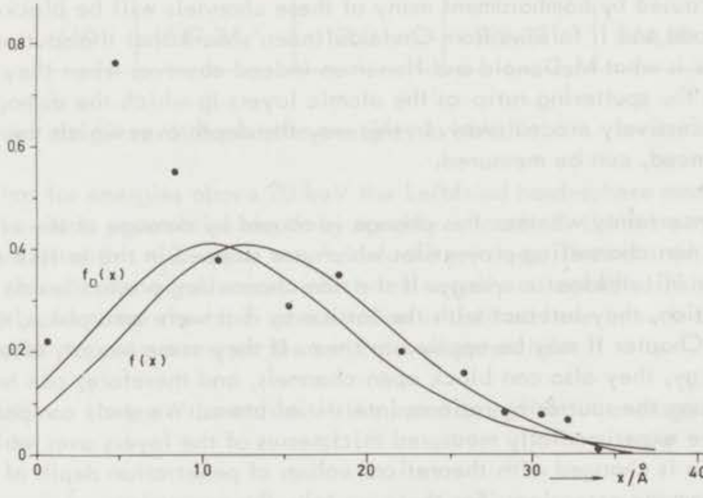

Fig. 7 Comparison of calculated range and damage distribution, f (x) and $f_D(x)$, with experimental results, obtained by 1 keV Kr^+ bombardment of Ge[25].

Finally we give a theoretical range and damage distribution, calculated with the help of an Edgeworth expansion (cf. Chapter II (2.43)) from first-, second- and third-order moments of the penetration depth x for 1 keV Kr^+-ions in Germanium, together with points measured by McDonald and Haneman. It is seen that there is a close agreement between range and damage distribution and a satisfactory agreement between the calculated and measured distributions for depthts above 10 Å (cf. fig. 7.

Ericsson et al.[29] have used proton channeling to estimate the depth of the damaged region in Si (cf. fig. 2 of this reference). This Si-target had been doped with 40 keV Sb-ions at room temperature. They concluded that the discorded region does not extend significantly beyond the depth of the implanted layer of Sb-ions. From $m_2/m_1 = 0.23$ and Fig. 5 we find $<x>/<x_D> = 1.18$ for $s = 2$ and 1.45 for $s = 3$. Taking account of the half-width of both distributions we find

$$\frac{<x> + <\Delta x^2>^{\frac{1}{2}}}{<x_D> + <\Delta x_D^2>^{\frac{1}{2}}} = \begin{matrix} 0.96 & s = 2 \\ 1.22 & s = 3 \end{matrix}$$

which is consistent with the experimental results.

Parsons and Balluffi[27] bombarded thin films of metastable amorphous Germanium with Xe^+-ions with energies from 20 to 160 keV. They observed crystallized regions in an electron microscope and determined the distribution of the apparent diameter of these regions. They observed that the most probable diameter is closely equal to the average range of the projectile measured along the path, which according to Lindhard[11] whould be about 20% greater than the average projected range $<x>$, which we have calculated. Assuming the crystallized regions to be identical with regions covered by collision cascades, we may identify the apparent cluster diameter with the transverse extension of the cascade, since the observations are made perpendicular to the ion beam direction. A good approximation for the transverse extension is given by

$$D = 2\sqrt{<y_D^2> + <z_D^2>} = 2\sqrt{2<y_D^2>} = \begin{matrix} 0.91 <x_D> & s = 2 \\ 0.98 <x_D> & s = 3 \end{matrix}$$

$<x_D>$ and $<y_D^2>$ are calculated with the help of the results of Chapter IV and Tables (5.2) for the energies used in this experiment. It turns out that the results do not agree with the experimental ones. The most probable diameter of the crystallized regions increases with the energy of the Xe^+-projectiles but much slower than is predicted by our theory.

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APPENDIX A

DERIVATION OF THE DIFFERENTIAL CROSS SECTION FOR AN INVERSE POWER POTENTIAL INTERACTION

Let us suppose that a particle with a kinetic energy in the keV range is scattered by a stationary one. If we want to calculate the differential cross section, we must start from a given interaction potential between them. For this we choose the general form of a screened Coulomb potential

$$V(r) = \frac{Z_1 Z_2 e^2}{r} U(r/a) \tag{A.1}$$

We consider the problem in center-of-mass co-ordinates and want to calculate the angle of deflection Θ as a function of the impact parameter p. To find a simple approximate result we shall use the momentum approximation, which means that the interaction of the moving particle with the stationary one is treated as a small perturbation on its initial motion, so that the deflection is assumed to be small and the path nearly rectilinear. If $K_\perp(x)$ denotes the component of the force, perpendicular to the rectilinear path at the point with distance x from the point of closest approach if there would have been no interaction (this point has the distance p from the scatterer) the deflection is given by

$$\Theta = \int_{-\infty}^{\infty} \frac{K_\perp(x)dx}{m_0 v^2} \tag{A.2}$$

where $m_0 = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass and v is the relative velocity.

$K_\perp(x)$ is given by

$$K_\perp(x) = -\frac{\partial V(r)}{\partial r} \cos\varphi \tag{A.3}$$

where $\cos\varphi = \frac{p}{r} = \frac{p}{\sqrt{p^2+x^2}}$

$K_\perp$ can be calculated explicitly by differentiating (A.1) with respect to r. We get then

$$K_\perp(x) = \left\{ \frac{Z_1 Z_2 e^2}{r^2} U(r/a) - \frac{Z_1 Z_2 e^2}{ra} U'(r/a) \right\} \cos\varphi \tag{A.4}$$

Hence

$$\Theta = \frac{Z_1 Z_2 e^2}{m_0 v^2} \int_{-\infty}^{\infty} dx \left\{ \frac{\cos^2\varphi}{p^2} U(p/a\cos\varphi) - \frac{\cos\varphi}{pa} U'\left(\frac{p}{a\cos\varphi}\right)\right\} \cos\varphi$$

(A.5)

$$= \frac{2Z_1 Z_2 e^2}{m_0 v^2} \int_0^{\frac{\pi}{2}} \cos\varphi d\varphi \left\{\frac{1}{p} U\left(\frac{p}{a\cos\varphi}\right) - \frac{1}{a\cos\varphi} U'\left(\frac{p}{a\cos\varphi}\right)\right\}$$

$$= \frac{b}{p} g\left(\frac{p}{a}\right)$$

where $g(y) = \int_0^{\pi/2} \cos\varphi d\varphi \left\{U\left(\frac{y}{\cos\varphi}\right) - \frac{y}{\cos\varphi} U'\left(\frac{y}{\cos\varphi}\right)\right\}$ and $b = \frac{2Z_1 Z_2 e^2}{m_0 v^2}$ is Bohr's collision diameter.

We now take for $U(r/a)$ the screening function, introduced in Chapter I.

(A.6) $$U(r/a) = \frac{k_s}{s}\left(\frac{a}{r}\right)^{s-1}$$

which is substituted in the expression for $g(p/a)$ which then becomes

(A.7) $$g(p/a) = \frac{k_s}{s} \int_0^{\pi/2} d\varphi \cos\varphi \cdot s \left(\frac{a\cos\varphi}{p}\right)^{s-1} = k_s \left(\frac{a}{p}\right)^{s-1} \int_0^{\pi/2} \cos^s\varphi \, d\varphi .$$

The integral in (A.7) is equal to the Beta function $\frac{1}{2} B\left(\frac{s+1}{2}; \frac{1}{2}\right)$ and is denoted by γ_s. Finally we obtain from (A.5) for the angle of deflection

(A.8) $$\Theta = b k_s a^{s-1} \gamma_s \frac{1}{p^s}$$

from which

(A.9) $$p = \left(\frac{b k_s a^{s-1} \gamma_s}{\Theta}\right)^{1/s}$$

We now introduce as a new variable the energy transfer in a collision, which is given by

(A.10) $$T = T_m \sin^2 \Theta/2 \quad \text{with } T_m = \frac{4m_1 m_2}{(m_1+m_2)^2} E.$$

As this treatment is based on the supposition that Θ is small, this relation can be replaced by

$$T = T_m \frac{\Theta^2}{4} \text{ or } \Theta = 2\left(\frac{T}{T_m}\right)^{\frac{1}{2}} \tag{A.11}$$

and this is substituted into (A.9), with the result

$$p = \left(\frac{b\,k_s\,a^{s-1}\,\gamma_s\,T_m^{\frac{1}{2}}}{2\,T^{\frac{1}{2}}}\right)^{1/s} \tag{A.12}$$

The differential cross section which is the probability that the moving particle will suffer a collision in which it transfers a kinetic energy between T and T + dT, can now be written as

$$d\sigma = \pi\, d\,(p^2) = \frac{\pi}{s}\left\{\frac{b^2\,k_s^2\,a^{2s-2}\,\gamma_s\,T_m}{4}\right\}^{1/s} \frac{dT}{T^{1+1/s}} \tag{A.13}$$

which is the result which we wanted to prove.

Though this result has been derived for soft collisions (i.e. small energy transfers and small deflections Θ) only, it turns out by comparison with exact cross sections that for small exponents s, the approximation is surprisingly good, even for head-on collisions. In the following table the results as calculated by Lindhard are given for different s, and $T = T_m$ (head-on collision)

s	1	1.5	2	3
$\frac{d\sigma(\text{exact})}{d\sigma(\text{Eq.(A.13)})}$	1	1.15	0.97	0.65

As the error, made in the momentum approximation is greatest for head-on collisions, we see that values of s between 1 and 2 provide an excellent approximation over the entire energy transfer interval. Also the case s = 3 may provide a better approximation than appears from this table, because head-on collisions are very improbable and do not have much weight in an averaging process over all possible collisions.

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APPENDIX B

DERIVATION OF EQUATION (2.7)

Our starting point is the equation

$$(2.4)\quad \eta \frac{\partial p}{\partial r} + \frac{1-\eta^2}{r} \frac{\partial p}{\partial \eta} = N \int_{\Delta}^{E} d\sigma' \left[p(r,\eta',E-T) - p(r,\eta,E) \right]$$

The meaning of the different symbols has been explained in the text.
We now want to substitute the expansion

$$(2.6)\qquad p(r,\eta,E) = \sum_{\ell=0}^{\infty} (2\ell+1) p_\ell(r,E)\, P_\ell(\eta) \quad .$$

We shall consider first the left-hand side of (2.4). This becomes

$$(B.1)\qquad \sum_{\ell=0}^{\infty} (2\ell+1)\, \eta \frac{\partial p_\ell}{\partial r} P_\ell(\eta) + \frac{1-\eta^2}{r} \sum_{\ell=0}^{\infty} (2\ell+1)\, p_\ell \frac{dP_\ell(\eta)}{d\eta}$$

To reduce this further, we use the recurrence relation

$$(B.2)\qquad (1-\eta^2) \frac{dP_\ell(\eta)}{d\eta} = \ell P_{\ell-1}(\eta) - \ell \eta P_\ell(\eta)$$

which yields on substitution into (B.1)

$$(B.3)\qquad \sum_{\ell=0}^{\infty} (2\ell+1)\, \eta \frac{\partial p_\ell}{\partial r} P_\ell(\eta) + \sum_{\ell=0}^{\infty} (2\ell+1) \frac{p_\ell}{r} \left[\ell P_{\ell=1}(\eta) - \ell\eta P_\ell(\eta) \right] \quad .$$

We now use another relation between the P_ℓ, namely

$$(B.4)\qquad (2\ell+1)\, \eta P_\ell(\eta) = (\ell+1) P_{\ell+1}(\eta) + \ell P_{\ell-1}(\eta) \quad .$$

The substitution of this relation in both the summations occurring in (B.3) gives the result

$$\sum_{\ell=0}^{\infty} \left\{ \ell P_{\ell-1}(\eta) + (\ell+1) P_{\ell+1}(\eta) \right\} \frac{\partial p_\ell}{\partial r} + \sum_{\ell=0}^{\infty} \left\{ \ell(\ell+1) P_{\ell-1}(\eta) - \ell(\ell+1) P_{\ell+1}(\eta) \right\} \frac{p_\ell}{r}$$

(B.5)

which is the left-hand side of Eq. (2.7). Consider now the right-hand side of (2.4), in which we shall write the differential cross section explicitly with the angular distribution as given in Eq. (1.5) and substitute (2.6). It then becomes (equal masses!)

$$\text{(B.6)}\quad N\int_{\Delta}^{E}\int_{-1}^{1}\int_{\sigma}^{2\pi} d\sigma\,\delta\left(\vec{n}\vec{n}' - \sqrt{\frac{E-T}{E}}\right) d(\vec{n}\vec{n}')\,\frac{d\varphi}{2\pi}\sum_{\ell=0}^{\infty}(2\ell+1)\Big[p_{\ell}(r,E-T)\,P_{\ell}(\eta') - p_{\ell}(r,E)\,P_{\ell}(\eta)\Big]$$

We now use the fact that η, η' and $\vec{n}\vec{n}'$ are connected through the cosine law of spherical trigonometry and use the addition theorem of the Legendre-polynomials which states for our case

$$\text{(B.7)}\quad P_{\ell}(\eta') = P_{\ell}(\eta)\,P_{\ell}(\vec{n}\vec{n}') + 2\sum_{m=1}^{\ell}\frac{(m-\ell)'}{(m+\ell)'}\,P_{\ell}^{m}(\eta)\,P_{\ell}^{m}(\vec{n}\vec{n}')\cos m\,(\varphi_2-\varphi_1)\quad .$$

Due to the fact that we have to integrate over φ_2 from 0 to 2π the summation over the associate polynomials disappears. As the value of $\vec{n}\vec{n}'$ is fixed by the δ-function we are left with

$$N\int_{\Delta}^{E} d\sigma\sum_{\ell=0}^{\infty}(2\ell+1)\left[p_{\ell}(r,E-T)\,P_{\ell}\left(\sqrt{\frac{E-T}{E}}\right)P_{\ell}(\eta) - p_{\ell}(r,E)\,P_{\ell}(\eta)\right]$$

which is the right-hand side of (2.7).

The derivation for the case of unequal masses proceeds in the same way. Only the deflection angle $\vec{n}\vec{n}'$ has a different value (cf. Chapter II).

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SUMMARY

In this thesis a theoretical treatment is given of the penetration depth of projectiles with kinetic energies in the keV region which enter into amorphous substances and of the collision cascades between target atoms, caused by them. In the latter case we have supposed the target material to be single- or polycrystalline.

In Chapter I we give a short review of previous work, done in these fields by various authors and we give the form of the interaction potential and of the differential cross-section on which the calculations in the following chapters are based. The potential is proportional to an inverse power of the interatomic distance with an exponent s between 2 and 4 and the corresponding differential cross-section is given by

$$d\sigma = C\, E^{-1/s} \frac{dT}{T^{1+1/s}}$$

where C is a proportionality factor, E the initial kinetic energy and T the energy transfer in the collision.

In Chapter II a theory of the penetration depth of projectiles in amorphous targets is developed. The theory is based on a balance equation which can be written for the function $p(\vec{r},\vec{n},E)$ which gives the probability density for a projectile with initial kinetic energy E and direction of motion $\vec{n}$ to come to rest at the point with vectorial coordinate $\vec{r}$ from the point of entrance as origin. It is possible to derive from this equation a recursion relation between the quantities $p_\ell^n(E)$ with different values of the indices n and ℓ. These quantities are linear combinations of moments of the penetration depth and of the projection of the total distance, reached by the projectile on the plane perpendicular to its initial direction of motion $\vec{n}$. The penetration depth is the projection of the total distance on $\vec{n}$, if $\vec{n}$ is normal to the target surface.
From this recursion relation all $p_\ell^n(E)$ with $n \geqq \ell$ and $n+\ell$ even can be calculated and from these the moments of all orders of the penetration depth can be found. These moments have been calculated for the case of ^{85}Kr-ions of various energies on amorphous Al_2O_3 and a cumulative distribution function has been constructed with the help of them. The theoretical results are compared with the experimental ones obtained by Domey and co-workers and the agreement is found to be satisfactory.

In Chapter III we consider the average number of recoils in a specified low-energy interval which occur in the collision cascade in single- or polycrystalline material, caused by an incoming projectile whose energy is supposed to be much greater than that of the recoils whose number is calculated. The calculation is performed for the cases that the projectile has the same mass and a different mass as the target atoms. It turns out that both cases give the same result. We have also calculated the variance of the recoil number. Also we have calculated the average sum of the momenta of all recoils in the energy interval considered.

In Chapter IV the spatial extension of the collision cascade is considered. With a method, analogous to the one used in Chapter II, the moments of the depth beneath the surface where recoils of a given energy are created, are calculated. This also had been done for the cases of the projectile having the same and a different mass as the target atoms.

In Chapter V some further details of the theoretical results are given. The ratio between the average depth of the penetration of the projectile and the average depth of the created damage is given for different power potentials and compared with an effective hard-sphere model. The same ratio is given for the second-order moments. Also are given the ratios between the variance of the penetration depths for different ratios between the masses of projectiles and target atoms for the case that $s = 2$, and for the equal mass case for $s = 1, 1\frac{1}{2}, 2, 3$ and 4.

The same ratios are given for the depth of the radiation damage created by the projectiles. These ratios are also compared with the hard-sphere model.
Then some theoretical results are compared with some experimental ones. Except in the case of the bombardment of a thin film, the agreement turns out to be satisfactory.

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SAMENVATTING

In dit proefschrift wordt een theoretische behandeling gegeven van de indringdiepte van projectielen met kinetische energie in het keV-gebied, die binnendringen in amorf materiaal en van de botsingscascades tussen targetatomen die door deze projectielen veroorzaakt worden. In dit laatste geval is het targetmateriaal één- of polykristallijn verondersteld.

In hoofdstuk I geven wij een kort overzicht van voorafgaand werk, op dit gebied verricht door andere auteurs en geven wij tevens de vorm van de wisselwerkingspotentiaal en van de differentiële werkzame doorsnede waarop de berekeningen in de volgende hoofdstukken gebaseerd zijn. Deze potentiaal is evenredig met r^{-s}, waarbij r de interatomaire afstand is en s ligt tussen 2 en 4 en de bijbehorende differentiele werkzame doorsnede wordt gegeven door

$$d\sigma = C\,E^{-1/s}\,\frac{dT}{T^{1+1/s}}\,,$$

waarin C een evenredigheidsfactor is, E de initiële kinetische energie en T de energie-overdracht in de botsing.

In hoofdstuk II wordt een theorie ontwikkeld over de indringdiepten van projectielen in amorf materiaal. Deze theorie is gebaseerd op een balansvergelijking, die kan worden opgeschreven voor de functie $p(\vec{r},\vec{n},E)$, die voor een projectiel met initiële kinetische energie E en bewegingsrichting $\vec{n}$, de waarschijnlijkheidsdichtheid representeert om tot rust te komen in het punt met coördinaatvector $\vec{r}$ van het punt van binnenkomst in het target als oorsprong. Het is mogelijk om uit deze vergelijking een recursiebetrekking af te leiden tussen de grootheden $p^n_\ell(E)$ met verschillende waarden van de indices n en ℓ. Deze grootheden zijn lineaire combinaties van momenten van de indringdiepte en van de projectie van de totale afstand, afgelegd door het projectiel op een vlak, loodrecht op de initiële bewegingsrichting $\vec{n}$. De indringdiepte is de projectie van de totale afstand op $\vec{n}$, als $\vec{n}$ loodrecht op het oppervlak van het target staat. Uit deze recursiebetrekking kunnen alle $p^n_\ell(E)$ met $n \geqq \ell$ en $n+\ell$ even berekend worden en hieruit weer de momenten van alle ordes van de indringdiepte. Deze momenten zijn berekend voor het geval van ^{85}Kr-ionen met verschillende energieën die binnendringen in amorf aluminiumoxyde (Al_2O_3), en een geïntegreerde verdelingsfunctie is geconstrueerd met behulp hiervan. De theoretische resultaten zijn vergeleken met experimentele, verkregen door Domey en medewerkers en de overeenstemming is bevredigend.

In hoofdstuk III beschouwen wij het gemiddelde aantal recoils in een gespecificeerd lage energie interval, die voorkomen in de botsingscascade in één- of polykristallijn materiaal, veroorzaakt door een projectiel waarvan de beginenergie verondersteld wordt veel groter te zijn dan die van de recoils waarvan het aantal berekend wordt. De berekening is verricht voor de gevallen dat de massa van het projectiel gelijk en ongelijk is aan die van de targetatomen. Beide gevallen geven hetzelfde resultaat. Ook de variantie van dit aantal is berekend. Verder is berekend de gemiddelde som van de impulsen van alle recoils in het beschouwde energie-interval.

In hoofdstuk IV wordt de ruimtelijke uitbreiding van de botsingscascade beschouwd. Met een methode, analoog aan die van hoofdstuk II, worden de momenten berekend van de diepte beneden het oppervlak waar recoils van gegeven energie worden gecreëerd. Ook dit is gedaan voor de gevallen dat het projectiel zowel gelijke als ongelijke massa heeft als de targetatomen.

In hoofdstuk V worden enkele verdere bijzonderheden van de theoretische resultaten gegeven. De verhouding van de gemiddelde indringdiepte en de gemiddelde diepte van de gecreëerde beschadiging wordt gegeven voor verschillende machtspotentialen en vergeleken met een effectief harde bollenmodel. Ook worden gegeven de verhoudingen van de variantie van de indringdiepte en het quadraat van de gemiddelde indringdiepte voor verschillende verhoudingen van de massa's van het projectiel en de targetatomen in het geval dat s = 2 en voor het geval van gelijke massa's voor de s-waarden 1, $1\frac{1}{2}$, 2, 3 en 4. Dezelfde verhoudingen worden gegeven voor de diepte van de veroorzaakte beschadiging. Deze verhoudingen worden ook met die van het harde-bollenmodel vergeleken.
Hierna worden enkele theoretische resultaten vergeleken met die van enkele experimenten. Behalve in het geval van het bombardement van een dunne laag blijkt de overeenstemming bevredigend.

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STELLINGEN

I

Neemt men in de in hoofdstuk III van dit proefschrift afgeleide resultaten de limiet E_f E_1, dan verkrijgt men de overeenkomstige resultaten, behorende bij amorf materiaal. Voor deze resultaten gelden dan echter niet meer de betrekkingen, die in het geval van kristallijn materiaal het behoud van energie en impuls uitdrukken.

Dit proefschrift, hoofdstuk III.

II

Het is mogelijk om de integraalvergelijking voor het gemiddelde aantal recoils in een botsingscascade, die een gegeven impuls verkrijgen, op te lossen, door een benadering voor de inhomogene term in deze vergelijking in te voeren.

Dit proefschrift, hoofdstuk III.

III

Het harde-bollen-model voor de interatomaire wisselwerking, zoals dat o.a. door Leibfried en Mika gebruikt is, geeft – voor de berekening van verdelingen van indringdiepten van projectielen in amorf materiaal – geen goede resultaten.

Dit proefschrift, hoofdstuk V,
G. Leibfried, Z.f.Phys. 171 1 1963,
G. Leibfried, K. Mika, Nukleonik 7 309 1965.

IV

De waarschijnlijkheid van omlading van een ion, gereflecteerd aan een metaaloppervlak, wordt beïnvloed door de atomaire structuur van dat oppervlak. De verklaring van Dahl voor dit verschijnsel is niet toereikend.

P. Dahl, Abstracts 8th Int. Conf. on Phen. in Ionized Gases, Wenen 1967, 51.
J.W. Gadzuk, Surface Science 6 133 1967.

V

De theorie van Martynenko, over de verstuivingsverhouding van éénkristallen als functie van de hoek met de normaal op het oppervlak van de invalsrichting der projectielen, bevat een tegenstrijdigheid.

Y.V. Martynenko, Sov.Phys. 6 1581 1965.

VI

De bewering van De Wames, Hall en Chadderton, dat de 'klassieke limiet' van de quantummechanische diffractietheorie voor door kristalvlakken gechannelde protonen een beter resultaat geeft dan de eenvoudige, klassieke theorie van Lindhard, wordt niet bevestigd door de experimenteel verkregen resultaten van Andersen, Davies, Nielsen en Andersen.

R.E. De Wames, W.F. Hall en L.T. Chadderton, te verschijnen.
J. Lindhard, Mat.Fys. Medd. Dan Vid Selsk 34 14 1965.
J.U. Andersen, J.A. Davies, K.O. Nielsen en S.L. Andersen, Nucl. Instr. 38 210 1965

VII

De door Peek bewezen aequivalentie tussen de 'sudden approximation' en de 1e Born-benadering met Hartree-Fock-golffuncties, is a priori duidelijk, evenals het feit, dat de toepasbaarheid van deze benaderingen twijfelachtig is.

J.M. Peek, Phys.Rev. 160 124 1967.

VIII

Het bezwaar, dat de Langmuir-Taylor-detector voor alkalibundels met energieeën hoger dan 3 eV minder effectief wordt, kan worden ondervangen door de functie van de ioniserende draad en de cylinder-collector te verwisselen.

S. Datz en E.H. Taylor, J.Chem.Phys. 25 389 1956.
E. Hulpke en C. Schlier, Z.f.Phys. 207 294 1967.

IX

In die magnetohydrodynamisch stabiele plasma-experimenten, waar het plasmaverlies uitsluitend bepaald wordt door het electrische veld in de grenslaag tussen magneetveld en plasma, is het principiëel onmogelijk deze verliezen tegen te gaan door met uitwendige hulpmiddelen te trachten dit electrisch veld te beïnvloeden.

X

Voor integrale geschiedschrijving, zoals door Jan Romein bedoeld, is de film als bronnenmateriaal van belang en wat betreft bepaalde aspecten van de 20^{e} eeuwse historie zelfs een essentieel onderdeel.

Jan Romein: Eender en Anders   Querido 1964.

Leiden, 14 februari 1968

J.B. Sanders

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