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Computer program for the evaluation of ion beam analysis energy spectra

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ABSTRACT

The computer program "SQUEAKIE" for evaluation of ion beam analysis (RBS or nuclear reaction) energy spectra is listed and described. Given an experimental energy spectrum in which the signals from all targetelements may be identified, this program directly yields the target stoichiometry versus depth from the surface. The program is based on solving an eigenvector problem by means of inverse iteration. The formalism, which has been derived in detail previously /1/, is briefly reviewed. Attempts to reduce computing time on small computers are discussed. On a large computer (Amdahl 470) typical CPU-times were $\sim$ 3 seconds per spectrum, on a smaller computer (NORD-100) $\sim$ 40 seconds.

CONTENTS

1. INTRODUCTION

The measurement of energy distributions of light ions emerging from a target during irradiation is widely used for microanalysis of solids /2-4/. The emerging ions result either from a nuclear reaction or from an elastic scattering process between an energetic light ion beam and the target atoms. The evaluation of sample composition versus depth from the energy spectra obtained from either process is formally very similar /5/.

Several procedures have been proposed for more or less automatic evaluation of such spectra, but most of them are not very good if more than 2 elements are present in the target.

One quite general formalism has been developed and described in detail /1/ which in principle may treat any number of targetelements. In the final approach one must here distinguish between cases where

a) for one of the target components the light ion yield is unknown,

or

b) the light ion yields from all target components may be distinguished.

The treatment of cases, where two or more signals are unknown is not possible without additional information. The procedure described for case a) has been modified to include the case of overlapping signals, i.e. two of the elemental signals are unknown, but their sum is measured /13, 14/.

The case b) is the more general one and very frequent in ion beam analysis experiments. A computer program, "SQUEAKIE", has been developed

for this case on the basis of the formalism of Reference 1. The program directly calculates the target composition vs. depth from experimental spectra. Together with Ref. 1 the present report provides a description and documentation of the program. Applications of "SQUEAKIE" have been published elsewhere /6-9, 14, 20/, and Chapter 7 includes a few more examples.

The type of experiment for which the program may be used is described in Chapter 2. The terminology of that Chapter is then used in the following. The program has presently been applied to RBS-spectra, whereas nuclear reaction energy spectra may pose some problems because of resolution effects. In a brief review of the formalism it is recalled how the target stoichiometry at a given depth may be calculated by solving an eigenvector problem.

Without consideration of the specific formalism, calculations, etc., Chapter 3 gives an overview of the function of the program. Even users who are not interested in the following chapters should at least look through this.

The calculation of the necessary physical quantities is discussed in Chapter 4. A simple description is given of the inverse iteration method for solving eigenvector problems (Sect. 4.4), and finally some general suggestions for optimizing the program are made.

The program itself is listed and described in Chapter 5. Extensively treated are the versions in Garching (Sects. 5.1-5.8). These Sections are not included in the present report, but reside on the Amdahl 470.

An updated listing of the sections may be obtained at any time directly from the authors. A version of "SQUEAKIE" modified for smaller computers (the NORD-100 in Aarhus) is discussed in Sect. 5.9.

The use of the program in Garching (including input and job control cards) is described in Chapter 6. It is recommended that all users study Sections 6.5 and 6.6 to avoid problems in interpreting results.

Users implementing versions of the program on other computers may benefit from the tests described in Section 7.1, when searching for programming errors. Together with Ref. 1 Section 7.2 describes tests of precision, stability, speed and applicability of the program as performed by the authors.

2. PRINCIPLE

The principles behind the program are primarily described for a Rutherford backscattering (RBS) measurement, but also the modifications necessary when nuclear reactions contribute are indicated.

2.1 Experiment

An RBS-experiment is illustrated in Fig. 1:

A beam of light ions with mass M_1 impinges on the surface of a solid target at an incident angle α to the surface normal (Fig. 1a). Penetrating the target the ions lose energy and the average inward energy $E(x)$ depends on depth x. Let us consider ions scattered through the angle θ at depth x by collision with a target atom of type 'i'. The

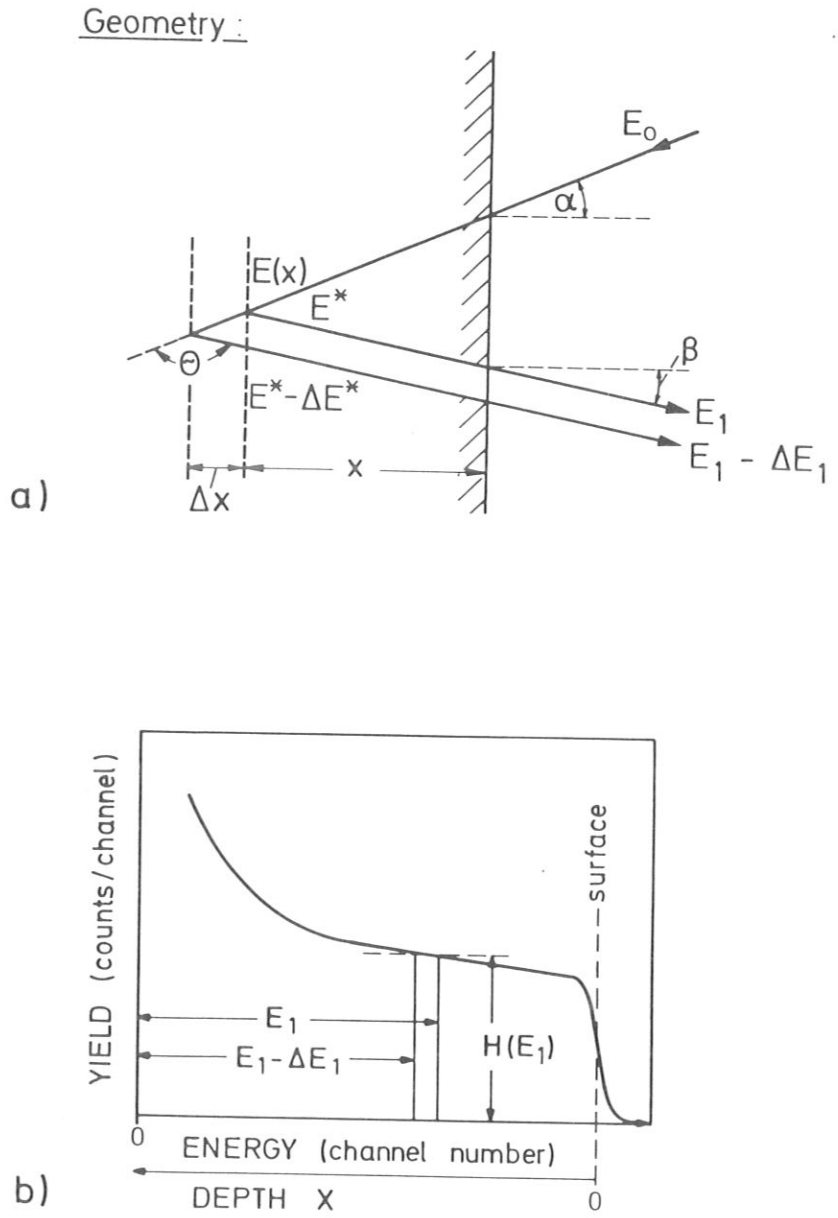


Fig. 1: Rutherford backscattering (RBS) measurement, see text.
a) Experimental geometry, b) Detected energy spectrum

energy $E_i^*(x)$ immediately after scattering depends on i and θ. Leaving the target at an angle ß to the surface normal the ions lose energy on the way out and are finally detected with energy $E_{1,i}(x)$.

In the case of nuclear reaction, the detected particles may be of a different type than the projectiles.

The detected energy spectrum (Fig. 1b) now may be evaluated with respect to type, depth and concentration of the element 'i'. In the following it is assumed, that the individual signals from the target components are identified, and the spectrum resides on a multi-channel analyser. It is important to limit the number of elements which may be present in the target, before using the program: Clearly the program may not distinguish between RBS-signals from a light element near the surface and a heavy element at larger depth. A larger number of possible elements therefore at best limits the depth of evaluation.

2.2 Formalism

i) RBS

The formalism needed for the above experiment is quite simple. Let us assume that we have already determined the target composition versus depth up to some depth x. At this depth let the target be composed of m elements with relative atomic concentrations $n_1, n_2, \ldots, n_m$, $(n_1+n_2+\ldots+n_m = 1)$, and atomic stopping powers $S^1, S^2, \ldots, S^m$.
Let us now consider projectiles backscattered from element 'i' through the angle θ in the depth-interval $[x, x+\Delta x_i]$. Δx_i is chosen, so that it corresponds to the energy width ΔE_1 of a channel in the experimental spectrum:

The average inward energy E varies between $E(x)$ and $E(x+\Delta x_i)$, and correspondingly the outward energy E_i^* immediately after scattering varies with depth. The precise functional relation between E_i^* and E (and i) is

described later. After escaping out through the target the scattered particles are finally detected with energies between $E_{1,i}(x)$ and $E_{1,i}(x)-\Delta E_1$. The energy $E_{1,i}(x)$ depends on element i and depth x, whereas the depth-interval Δx_i is related to i and the energy difference ΔE_1 through /3/

$$\Delta E_1 = \Delta x_i \cdot dE_{1,i}/dx \tag{2.1}$$

As ΔE_1 is a constant, Δx_i will in general vary with i. If this was not so, we could directly determine the relative concentrations n_i from the numbers H_i of detected particles in each channel:

$$H_i(E_{1,i}) = n_i(x) \cdot \left(\frac{d\sigma}{d\Omega}\right)_i \cdot N_{prim} \cdot \Delta\Omega \cdot \frac{\Delta x_i}{\cos\alpha} \tag{2.2}$$

where $\left(\frac{d\sigma}{d\Omega}\right)_i$ is the differential scattering cross section, N_{prim} is the primary beamdose (ions/cm^2), and $\Delta\Omega$ is the detector acceptance solid angle.

As it is, the estimate

$$(n_1:n_2:\ldots:n_m) \sim \frac{H_1}{\left(\frac{d\sigma}{d\Omega}\right)_1} : \frac{H_2}{\left(\frac{d\sigma}{d\Omega}\right)_2} : \ldots : \frac{H_m}{\left(\frac{d\sigma}{d\Omega}\right)_m} \tag{2.3}$$

still provides a very good start 'guess' for our iteration (see later). We shall (later) see examples of the variation of Δx_i with i.

For now, we factorize the derivative $(dE_{1,i}/dx)$ of eq. (2.1) as

$$dE_{1,i}/dx = S_{c,i}(E) \cdot e_i(E_i^*, E_{1,i}, x) \tag{2.4}$$

where the general energy loss factor at depth x

$$S_{c,i}(E) = dE_i^*/dx \tag{2.5}$$

may be expressed as composed of contributions from the stopping before and after the collision

$$S_{c,i}(E) = \frac{\partial E_i^*}{\partial E} \frac{S(E)}{\cos\alpha} + \frac{S(E_i^*)}{\cos\beta} \tag{2.6}$$

Here S(E') is the average <u>total</u> stopping power at energy E' and depth x.

The factor

$$e_i(E_i^*, E_{1,i}, x) = \frac{dE_{1,i}}{dE_i^*}(x) \tag{2.7}$$

enters because of the energy dependence of the stopping power: Two projectiles leaving the same depth x with an energy difference dE* will reach the surface with an energy difference dE_1, which is not exactly the same as dE*. The factor is calculated in each depthstep.

Assuming linear additivity of the atomic stopping powers (Bragg's rule) we have

$$S(E) = \sum_{j=1}^{m} (n_j \cdot S^j(E)) \tag{2.8}$$

which inserted in eq. (2.6) gives

$$S_{c,i}(E) = \sum_{j=1}^{m} (n_j \, a_{ij}) \tag{2.9}$$

Here the coefficients a_{ij} are defined by

$$a_{ij} = \left(\frac{dE_i^*}{dE}\right) \cdot \frac{S^j(E)}{\cos \alpha} + \frac{S^j(E_i^*)}{\cos \beta} \qquad (2.10)$$

From eqs. 2.1, 2.4 and 2.9 we thus get

$$\Delta x_i = \Delta E_1 / \{e_i \cdot \sum_{j=1}^{m} (n_j \, a_{ij})\} \qquad (2.11)$$

and inserting this in eq. 2.2 and rewriting, we finally end up with the eigenvector problem /1/

$$\underline{\underline{D}} \, \underline{n} = Q \, \underline{n} \qquad (2.12)$$

where the matrix $\underline{\underline{D}} \equiv (C_i \, a_{ij})$, the eigenvector $\underline{n} \equiv (n_1, n_2, \ldots, n_m)$, the eigenvalue $Q \equiv N_{prim} \, \Delta\Omega$ and

$$C_i \equiv \frac{H_i \cdot \cos\alpha \cdot e_i}{\left(\frac{d\sigma}{d\Omega}\right)_i \, \Delta E_1} \qquad (2.13)$$

Thus, the matrix $\underline{\underline{D}}$ is easily calculated from known quantities.

ii) Nuclear reaction analysis

The evaluation of the energy spectra obtained from nuclear reactions is formally very similar to the above /5/. The major difference is that the detected particles may be of a different type than the projectiles. In the above formalism this simply means that we must distinguish bet-

ween the atomic stopping powers S_p^j for the projectiles, and those (S_d^j) for the detected particles. It is then sufficient to modify eq. 2.10 to

$$a_{ij} = \left(\frac{\partial E_i^*}{\partial E}\right) \cdot \left(\frac{S_p^j(E)}{\cos \alpha}\right) + \frac{S_d^j(E_i^*)}{\cos \beta} \qquad (2.10')$$

Of course, in the actual program this requires a few more changes. Thus the factor $(\partial E_i^*/\partial E)$ now becomes somewhat more complicated /5/, and an analytical expression for the reaction cross section must be known $(d\sigma/d\Omega)_i$.

The typical application of the present method for nuclear reaction analysis would actually involve signals from both backscattering and nuclear reaction. It is not easy to design a program for general use in such experiments, as a variety of other considerations may play in, notably the quite different depth resolutions for RBS and nuclear reaction analysis. Quite often one might also wish to exploit some previous knowledge of the target composition: When nuclear reaction analysis is employed to determine the depth distribution of a light implant, we usually know the stoichiometry of the substrate before implantation! The description below should enable the reader to modify the program for his own purpose.

2.3 Is this program really necessary?

As mentioned above, the simple estimate (eq. 2.3) would be sufficient, if only Δx_i (eq. 2.2) did not depend on the element 'i'. It is therefore quite reasonable to ask whether Δx_i really does vary so much with i, that it justifies all the present work. Let us look briefly into this:

Comparing eqs. 2.1 and 2.4 we see that the element dependence of Δx_i is caused primarily by the corresponding variation of $S_{c,i}(E)$ with i. From eq. 2.6 we see that $S_{c,i}(E)$ depends on i in two ways - directly via the factor $(\partial E_i^*/\partial E)$ and indirectly because $S(E_i^*)$ varies with E_i^*. For a given set of target elements we shall therefore expect the strongest dependence in the energy region where the stopping varies fastest with energy. For RBS-experiments we thus find a significant effect for 1-2 MeV $^4He^+$-beams.

For the somewhat special case of 1.5 MeV $^4He^+$-ions backscattered from a thin Pt-film on BeO, we find a Δx_{Pt} which is almost twice as large as Δx_{Be}. The study of CuO_x-films on BN-substrates, however, has been of considerable interest in corrosion studies /7/, and here Δx_B and Δx_O would be of the order of 70 % and 80 % of Δx_{Cu}, only.

For experiments involving nuclear reactions considerably larger variations of Δx_i are possible.

Now,whether the present program is really necessary thus depends on the desired accuracy. Experience shows that for most applications until now /6-9, 14, 20/, the use of eq. 2.3 alone would typically lead to errors of 25 % or more in the estimate of relative concentrations $(n_i:n_j)$, even without the influence of statistical effects. In contrast, inverse iteration following such an initial estimate would effectively eliminate these errors.

3. FUNCTION

Let us first consider the structure of the program in general, the application of the inverse iteration, and the principles behind the two independent estimates of the total content of each element. A few details are discussed in Section 3.4, notably the choice of depth step and stop criteria, whereas the actual calculations are described in Chapter 4.

3.1 Stoichiometry vs. depth

1. The program starts with identifying the surface signals from the m_e possible target elements. Some of these may be zero or negligible, indicating that the corresponding elements are not present at the surface. A pointer is introduced, indicating only those elements yielding a significant contribution (estimated $> 10^{-3}$) in the order given by the element list in the input. From the non-zero signals the surface composition of the target is evaluated (by inverse iteration).

2. A depth step Δx_o is chosen, within which the target composition is assumed to remain constant. This step is chosen to correspond approximately to the width of a channel in the last of the non-zero signals (indicated by the pointer,above). It will thus usually correspond to somewhat more or less than a channel in the other elemental signals (see Section 3.4).

3. From the 'known' composition (evaluated above) the energy losses within this depth step are calculated, and the elemental signals from depth Δx_0 are identified. Simultaneously the factors $e_i(\Delta x_0)$ of eq. 2.7 are estimated numerically. From the non-zero signals the composition of the target is evaluated at depth Δx_0 (compare above).

4. The next depth step Δx_1 is chosen so that it corresponds approximately to the width of a channel in the last of the non-zero signals from depth Δx_0 (indicated by the pointer). We note that this signal may originate from another element than the one used for choosing Δx_0 above. The target composition just derived for depth Δx_0 is assumed to remain constant in the interval $[\ \Delta x_0,\ \Delta x_0+\Delta x_1]$.

5. From the 'known' compositions of both depth steps the necessary energy losses are calculated, and the elemental signals from depth $\Delta x_0 + \Delta x_1$ are identified. Simultaneously the factors $e_i(\Delta x_0+\Delta x_1)$ are estimated. From the non-zero signals the composition of the target is evaluated at depth $\Delta x_0 + \Delta x_1$,

   and so forth ...

3.2 Inverse iteration vs. depth

1. In each depth step the local stoichiometry is evaluated from the corresponding experimental yields by inverse iteration. The formalism does not allow for non-contributing elements (yield $H_i \simeq 0$). This was the reason for introducing the pointer

(Sect. 3.1) selecting only those elements yielding a significant contribution.

2. The inverse iteration requires an 'initial guess' of both eigenvector $\underline{n}$ and eigenvalue Q. Here $\underline{n}$ is estimated by means of eq. 2.3, i.e. an estimate which may be quite imprecise at larger depths (see Sect. 2.3). However, as demonstrated in Sect. 7.2 even very crude estimates of $\underline{n}$ are more than sufficient for a very fast iteration.
Correspondingly, Q_o is estimated from the 'initial guess' (eq. 2.3): Inserting eq. 2.2 in eq. 2.9, taking all depth-intervals Δx_i to be equal, substituting eq. 2.1 and finally eq. 2.4, we get the factor

$$D_{ef} \equiv \sum_j \{e_i \cdot a_{ij} H_j/(\frac{d\sigma}{d\Omega})_j\} \cong Q \cdot \Delta E_1/\cos \alpha \qquad (3.0)$$

As D_{ef} may in principle be determined, we have then an estimate for $Q \equiv N_{prim}\Delta\Omega$.

3. Along with an iterated eigenvector $\underline{n}$, the inverse iteration also yields an improved estimate of Q in each depth step. This value is tabulated together with the stoichiometry vs. depth for various purposes (see Sects. 3.3, 5.9 and 7.2).

3.3 Integrated contents vs. depth

For a given depth x, the integrated content Int(i,x) of an element i is the total areal density (atoms/cm^2) of the element between the surface and the depth x.

The program has facilities to print two independent estimates of Int(i,x) vs. x for all i. None of these are particularly related to the formalism of Ref. 1. For further details see below and Sect. 7.2.

1. Assume that we have already calculated the stoichiometry vs. depth up to a given depth x. We then have a list of depth steps containing for the individual step 'j' the length Δx_j (in atoms/cm^2) and the relative contribution n_i for each element i. It is thus straightforward to add up these contributions from the surface up to the depth x:

$$\mathrm{Int}(i,x) = \sum_{j=o}^{k} n_j \cdot \Delta x_j \qquad (3.1)$$

We recall that $\sum_{i=1}^{m} n_i = 1$ (Sect. 2.2), and of course $\sum_{j=o}^{k} \Delta x_j = x$.

2. A quite independent approach is particularly suited for thin layers, e.g. contaminations on a surface, etc. In the so-called 'Thin Film Approximation' the <u>total</u> scattering yield from a thin film of thickness d_i (atoms/cm^2) is given by /3/

$$A_i = N_{prim}\, \Delta\Omega \left(\frac{d\sigma}{d\Omega}\right)_i \cdot d_i/\cos\alpha \qquad (3.2)$$

where the scattering cross-section $(d\sigma/d\Omega)_i$ is evaluated for the beamenergy. The approximation breaks down for film thicknesses

so large, that the inward energy loss in passing d_i causes a significant variation in $(d\sigma/d\Omega)_i$. In the present program the approximation is extended to slightly larger d_i by evaluating $(d\sigma/d\Omega)_i$ for the average energy between the primary E_o and the energy $E(d_i)$ after passage of d_i.

While stepping in through the target, calculating stoichiometry vs. depth (above), the program calculates also the values of A_i for each depth step: Since the elemental signals corresponding to each step are identified anyway, it is simple to simultaneously add up the signals originating between the surface and the present depth, for each element. Clearly, this does not work if part of the targetcomposition was already evaluated from a previous spectrum (see below).

A particular problem is the question of resolution effects /1/. Due to the finite experimental resolution, part of the signals are usually smeared so that they extend to channels above the 'ideal surfacechannels'. For very thin films up to half of the resulting peak may appear to originate from 'negative depths'. In summing up the <u>total</u> yield it is therefore necessary to specify how many channels above the surfacechannels are to be included. In the present program this is done by giving the FWHM of the experimental resolution at the surface (in number of channels) in the input.

In each depthstep the quantity

$$d_i \cdot N_{prim}\,\Delta\Omega = A_i \cos\alpha/(\frac{d\sigma}{d\Omega})_i \qquad (3.3)$$

is calculated, and this is the quantity listed vs depth later. It remains for the user to decide whether he will then take the factor $N_{prim}\,\Delta\Omega$ from the listed eigenvalues Q (above) or determine it otherwise experimentally.

3.4 Details

a) Choice of depthstep

The results are quite insensitive to the length of the depthstep, as long as it does not correspond to several channels in some signals. For normal use there is nothing gained by choosing steplengths corresponding to less than a channel in all the signals (see also b. Interpolation between channels). The program chooses a steplength Δx_s corresponding approximately to one channel (i.e. to the detected energy interval ΔE_1) in one of the signals:

For the signal from scattering on element i we calculate the corresponding general energy loss factor $S_{c,i}(E(x))$ of eq. 2.6. This is a crude approximation of the derivative $dE_{1,i}/dx$ (see eq. 2.4), so we may use the estimate

$$\Delta x_s = \Delta E_1 / S_{c,i}(E(x)) \tag{3.4}$$

for this depthstep.

b) Interpolation between channels

In general the ideal signals arising from a given depth do not correspond to an integral channel number for all elements. However, the discreteness induced by collecting a continuous energy spectrum in a finite number of channels is physically meaningless, and we introduce no additional error by interpolating linearly between channels.

c) Results from previous spectra

The optimum experimental parameters for determining depth distributions depend on the depths to be analysed. Thus, for a given target we may wish to improve the depth resolution at the surface by tilting the target (perhaps to $\alpha \sim 80^{o}$ /10/), but this would be detrimental to signals arising from 'large' depths. One might then try to combine the results from two or more spectra obtained with various angles of incidence. Or we may need several different measurements in order to separate the elemental signals from various depths. Therefore the program allows a table to be read in from a file, listing target composition vs. depth as calculated from a previous spectrum. This list is now taken as specifying a number of depthsteps of 'known' composition, up to the maximum listed depth x_m.

Before evaluating the present spectrum, the program now calculates the corresponding inward beam energy $E(x_m)$, and then proceeds as above:

The next depthstep Δx_j is chosen, and the target composition taken as constant between x_m and $x_m + \Delta x_j$. From this the energy losses in this depthstep are calculated. From the above list furthermore the outward energy losses are calculated, stepping out through the target. Thus the elemental signals from depth $x_m + \Delta x_j$ are identified in the present spectrum, and so forth ...

d) Stop-criteria

A weakness of the original version (Sects. 5.1-5.7) is the difficulty in defining a reasonable 'stop-criterium'. We must somehow specify when the evaluation of a spectrum should be terminated, so that elemental signals are still distinguished: If the program proceeds to sufficiently large depths, it may eventually encounter again the surface signals originating from a light element, and now interpret this as the signal from a heavier element at large depth (see Sect. 2.1).

This problem is automatically avoided in the alternative version (Sect. 5.8) and in the Aarhus-version (Sect. 5.9) by the use of element 'markers', which however limits the applicability for some purposes.

In the original version the stop-criteria are problematic: One either specifies the minimum inward beam-energy 'EMIN', or the lowest channelnumber 'NCHMIN' to be evaluated (Sect. 5.1). The program progresses stepwise from the target surface towards larger depths x, calculating the stoichiometry (Sect. 3.1). In each step the inward beamenergy E(x) is calculated, and the corresponding channels in the detected energy spectrum are identified. The evaluation of the spectrum is terminated, when either i) $E(x) < EMIN$, or ii) a channelnumber below NCHMIN is to be evaluated.

These options are obviously not very good, except perhaps in routine evaluation of many similar spectra. One may often have to evaluate a spectrum twice, or evaluate it up to too large depths. A study of the printed output (Sect. 6.4) is usually necessary (see also Sect. 6.6).

4. CALCULATIONS

Below the calculation of the various quantities entering the formalism is discussed. A simple description is given of the inverse iteration method, sufficient for understanding the quite simple calculations used in the present program, whereas more sophisticated versions are available in the literature. Finally, in Section 4.5 a few general suggestions are made for optimizing the program. Such optimizations are discussed for an actual program version in Section 5.9.

4.1 Scattering/reaction - cross section

i) RBS

Rutherford Backscattering Spectrometry /3/ is based on the Rutherford scattering cross section for projectiles of mass M_1 incident on targetatoms of mass M_i:

$$\frac{d\sigma}{d\Omega} R = \frac{Z_1^2 Z_i^2}{E^2} \frac{e^4}{16} f(\theta) \qquad (4.1)$$

where

$$f(\theta) = \frac{4}{\sin^4\theta} \frac{\{\cos\theta + g(\theta)\}^2}{g(\theta)} \qquad (4.2)$$

and

$$g(\theta) = \sqrt{1 - M_1^2 \sin^2\theta / M_i^2} \qquad (4.3)$$

Andersen et al. /15/ present a thorough discussion of the Rutherford scattering cross section and various analytical screening corrections for the energies and angles of interest here, and conclude that the factor

$$\frac{d\sigma_S}{d\sigma_R} = \left\{ \frac{1 + \frac{1}{2}\frac{V_1}{E_{cm}}}{1 + \frac{V_1}{E_{cm}} + \left(\frac{1}{2}\frac{V_1}{E_{cm}}\frac{1}{\sin\frac{\theta}{2}}\right)^2} \right\}^2 \qquad (4.4)$$

can be used to describe backscattering results within 1 %. E_{cm} is the center-of-mass energy, and we approximate $V_1 \simeq 49 \cdot Z_1 \cdot Z_2^{4/3}$ eV (static screening?). At MeV-energies where $V_1/E_{cm} << 1$ we can then estimate

$$\frac{d\sigma_S}{d\sigma_R} \simeq \left\{ \frac{1 + 24.5\,\frac{Z_1\,Z_2^{4/3}}{E}}{1 + 49\,\frac{Z_1\,Z_2^{4/3}}{E}} \right\}^2 \qquad (4.5)$$

for light ions. Finally we note, that if E is expressed in eV, then

$$\frac{d\sigma_R}{d\Omega} = \frac{Z_1^2\,Z_i^2}{E^2}\, f(\theta) \cdot 1.296 \cdot 10^{-15}, \text{ in cm}^2 \qquad (4.6)$$

ii) Nuclear reaction

For nuclear reaction analysis the differential cross section is usually not known as well as for RBS. In view of the remarks of Section 2.3 the present formalism is often only superior to a simple estimate (eq. 2.3) if the absolute cross section ($d\sigma/d\Omega$) is known to better than $\sim$ 25 %. For the $^3He(d,p)^4He$-reaction, for instance, such an accuracy has only been obtained quite recently /16/.

4.2 Scattering/reaction - energies

i) RBS

For elastic scattering of projectiles of mass M_1 on atoms of mass M_i conservation of energy and momentum give

$$E_i^* = K_i \cdot E \tag{4.7}$$

where the kinematic recoil factor /3/

$$K_i = \left\{\frac{M_1 \cos\theta}{M_1+M_i} + \left[\left(\frac{M_1}{M_1+M_i}\cos\theta\right)^2 + \frac{M_i-M_1}{M_1+M_i}\right]^{1/2}\right\}^2 \tag{4.8}$$

θ is the scattering angle.

In this case, furthermore, the derivative

$$\partial E_i^*/\partial E = K_i \tag{4.9}$$

so this is a useful constant to calculate once and for all.

We note for later use (Function XK) that a negative argument under the square-root corresponds to a scattering angle θ which is not possible for the given projectile-target combination. This is for instance encountered if the program attempts backscattering of ^{4}He-ions from H-atoms in the target!

ii) Nuclear reaction

If the projectiles (mass M_1) undergo some nuclear reaction (energy release $\tilde{Q}$) with a target atom of mass M_i resulting in a detected particle (mass M_3) and another particle (mass M_4) the energy E_i^* of the detected particle immediately after reaction is instead /5/

$$E_i^* = \frac{M_4}{M_3+M_4}\,\tilde{Q} + \frac{E}{(M_3+M_4)^2}\,f\,(M_j,\ \theta,\ E,\ \tilde{Q}),\ j = 1,\ 3,\ 4 \qquad (4.10a)$$

where

$$f = 2M_1M_3\cos^2\theta + (M_3+M_4)(M_4-M_1) + 2\cos\theta g^{1/2}(M_j,\theta,E,\tilde{Q}) \qquad (4.10b)$$

and

$$g = M_1^2\,M_3^2\cos^2\theta + M_1M_3(M_3+M_4)(M_4-M_1) + M_1M_3M_4(M_3+M_4)\,\frac{\tilde{Q}}{E} \qquad (4.10c)$$

In this case the derivative $\partial E_i^*/\partial E$ is also a function of energy E:

$$\partial E_i^*/\partial E = \frac{f}{(M_3+M_4)^2} - \frac{M_1M_3M_4}{M_3+M_4}\,\frac{\tilde{Q}}{E}\cdot g^{-1/2}\cos\theta \qquad (4.11)$$

4.3 Stopping power

i) In the original program the stopping power is calculated using the formula

$$S(E) = \frac{S_{High}\cdot S_{low}}{S_{High} + S_{low}} \qquad (4.12a)$$

where

$$S_{low} = \varepsilon_1\cdot E^{\varepsilon_2} \qquad (4.12b)$$

and

$$S_{High} = (\varepsilon_3/E)\ln\left[1 + \frac{\varepsilon_4}{E} + \varepsilon_5\cdot E\right] \qquad (4.12c)$$

E is the energy in keV.

This formula is meant to use the coefficients of the semi-empirical stopping powers of Ziegler /11/ and Andersen and Ziegler /12/ for He- and hydrogen ions. A few modifications are necessary, though:

For He-projectiles E should be replaced by E/1000 in S_{High}.

For ^{3}He-ions or deuterons S(E) is evaluated as the stopping power of ^{4}He-ions or protons, respectively, at the same velocity. This is remedied by defining the energy scaling factor FE as 1.0 for protons and ^{4}He-ions, 4/3 for ^{3}He-ions and 0.5 for deuterons. Then the stopping power for any of the isotopes at energy E equals S(FE E).

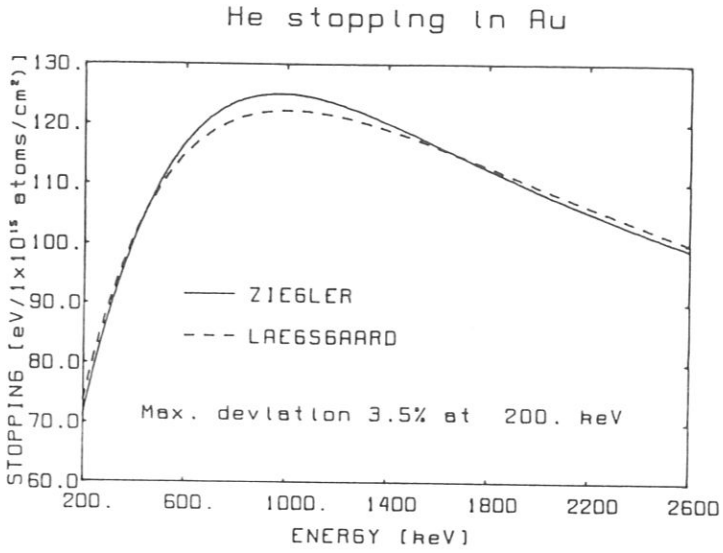
ii) The expression (4.12) is quite complicated and time-consuming to calculate, especially on a smaller computer. For the version used on the NORD-100 in Aarhus computertime was reduced using an existing stopping power subroutine /17/ based on the expression

$$S(E) = \varepsilon_a \cdot \sqrt{E}/(1 + \varepsilon_b \sqrt{E} + \varepsilon_c E) \qquad (4.13)$$

The constants ε_a, ε_b and ε_c have been determined from a least squares fit to the semiempirical helium stopping power of Ziegler /11/ in the energy range 0 to 4 MeV.

This expression is considerably faster to calculate than (4.12), particularly on small computers (see Section 4.6). The goodness of the least squares fit and the accuracy of the stopping power expression (4.13) can be judged by a comparison to the Ziegler values /11/. Figure 2 shows typical examples of such a comparison: For energies higher than $\sim$ 200 keV

a)



b)

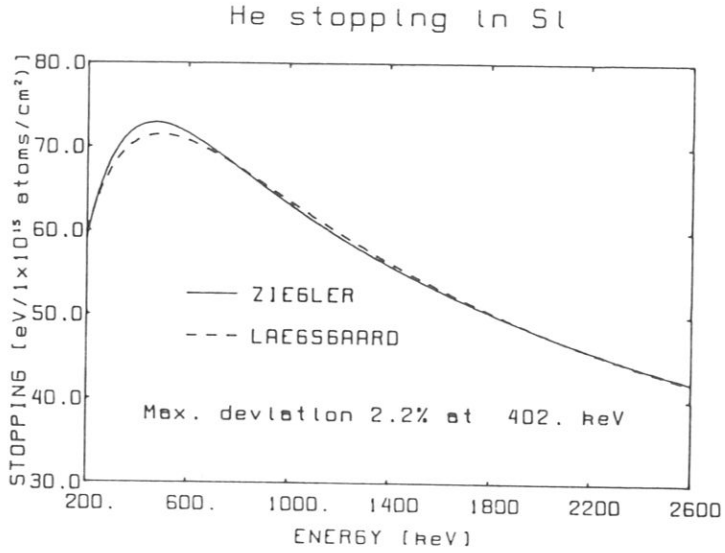


Fig. 2: Comparison of ^{4}He-stopping power expressions. Solid line semiempirical expression (Eq. 4.12) from Ref. 11; broken line-fit to this expression (eq. 4.13). Note suppressed zero on axis.

a) ^{4}He stopping power in Au, 200-2600 keV.

b) ^{4}He stopping power in Si, 200-2600 keV.

the expression (4.13) reproduces stopping power values very well, and the overall accuracy is clearly within the experimental uncertainties /11/. The accuracy is generally worst at the low energy end (see Fig. 2a).

4.4 Inverse Iteration

Inverse iteration is a powerful and accurate technique for the computation of the eigenvector $\underline{s}_r$ corresponding to a given eigenvalue Q_r. The method is usually very economical, and yields, as a byproduct, also an improved value for Q_r. A detailed account is given in Ref. 18, but we have found it appropriate to include at least a simplified description here also.

i) Principle

We are giving the (mxm)-matrix $\underline{\underline{D}}$, which has the eigenvectors $\underline{s}_j$ and the eigenvalues Q_j, where $j = 1,2,\ldots,m$. We want the eigenvector $\underline{s}_r$ corresponding to some eigenvalue Q_r:

$$\underline{\underline{D}} \cdot \underline{s}_r = Q_r \cdot \underline{s}_r \qquad (4.14)$$

The vector $\underline{s}_r$ is totally unknown, and only a very rough guess of Q_r is available.

We need to assume that

a) the eigenvectors $\underline{s}_j$ form a basis in C^m (all the eigenvalues are different from each other), and

b) our initial guess, Q_o, is closer to Q_r than to any other eigenvalue, but $Q_o \neq Q_r$.

In reality we have always yet found these assumptions to hold (see below).

Then inverse iteration yields the eigenvector $\underline{s}_r$ and a better estimate of Q_r:

$\underline{s}_r$ is a solution to the singular system of equations (4.14)

$$\underline{\underline{B}}\ \underline{s}_r = \underline{0} \tag{4.15}$$

where

$$\underline{\underline{B}} = (\underline{\underline{D}} - Q_r\ \underline{\underline{I}}) \tag{4.16}$$

and $\underline{\underline{I}}$ is the unit matrix. From assumption b above, then, the matrix

$$\underline{\underline{B}}_0 = (\underline{\underline{D}} - Q_0\ \underline{\underline{I}}) \tag{4.17}$$

is regular, so the equation

$$\underline{\underline{B}}_0\ \underline{y}_k = \underline{y}_{k-1} \tag{4.18}$$

has precisely one solution for a given $\underline{y}_{k-1}$, namely the vector

$$\underline{y}_k = \underline{\underline{B}}_0^{-1}\ \underline{y}_{k-1} \tag{4.19}$$

This is then used to define an iteration process, starting with some non-zero vector $\underline{y}_0$ ($k = 1$), and we may show this to converge towards the direction of $\underline{s}_r$.

For this purpose we note first, that for any eigenvector $\underline{s}_i$

$$\underline{\underline{D}}\ \underline{s}_i = Q_i\ \underline{s}_i \Rightarrow (\underline{\underline{D}}-Q_0\underline{\underline{I}})\underline{s}_i = (Q_i-Q_0)\underline{s}_i$$

$$\Rightarrow \underline{\underline{B}}_0^{-1}\ \underline{s}_i = (Q_i-Q_0)^{-1}\ \underline{s}_i \tag{4.20}$$

Now, from assumption a we know that any vector $\underline{y}_o$ may be written as a sum

$$\underline{y}_o = d_1 \underline{s}_1 + d_2 \underline{s}_2 + \ldots + d_m \underline{s}_m \qquad (4.21)$$

and we may easily choose a start vector, $\underline{y}_o$, with a component along the basis (eigen) vector $\underline{s}_r$ ($d_r \neq 0$) - for instance $\underline{y}_o = (1,1,\ldots,1)$.

Inserting eq. (4.21) in (4.19) we get first

$$\underline{y}_1 = \sum_{l=1}^{m} d_l \underline{\underline{B}}_o^{-1} \underline{s}_l \qquad (4.22)$$

and thus, from (4.20)

$$\underline{y}_1 = \sum_{l=1}^{m} \frac{d_l}{(Q_l - Q_o)} \underline{s}_l \qquad (4.23)$$

Repeated use of (4.19) then leads to

$$\underline{y}_k = \sum_{l=1}^{m} \frac{d_l}{(Q_l - Q_o)^k} \underline{s}_l =$$

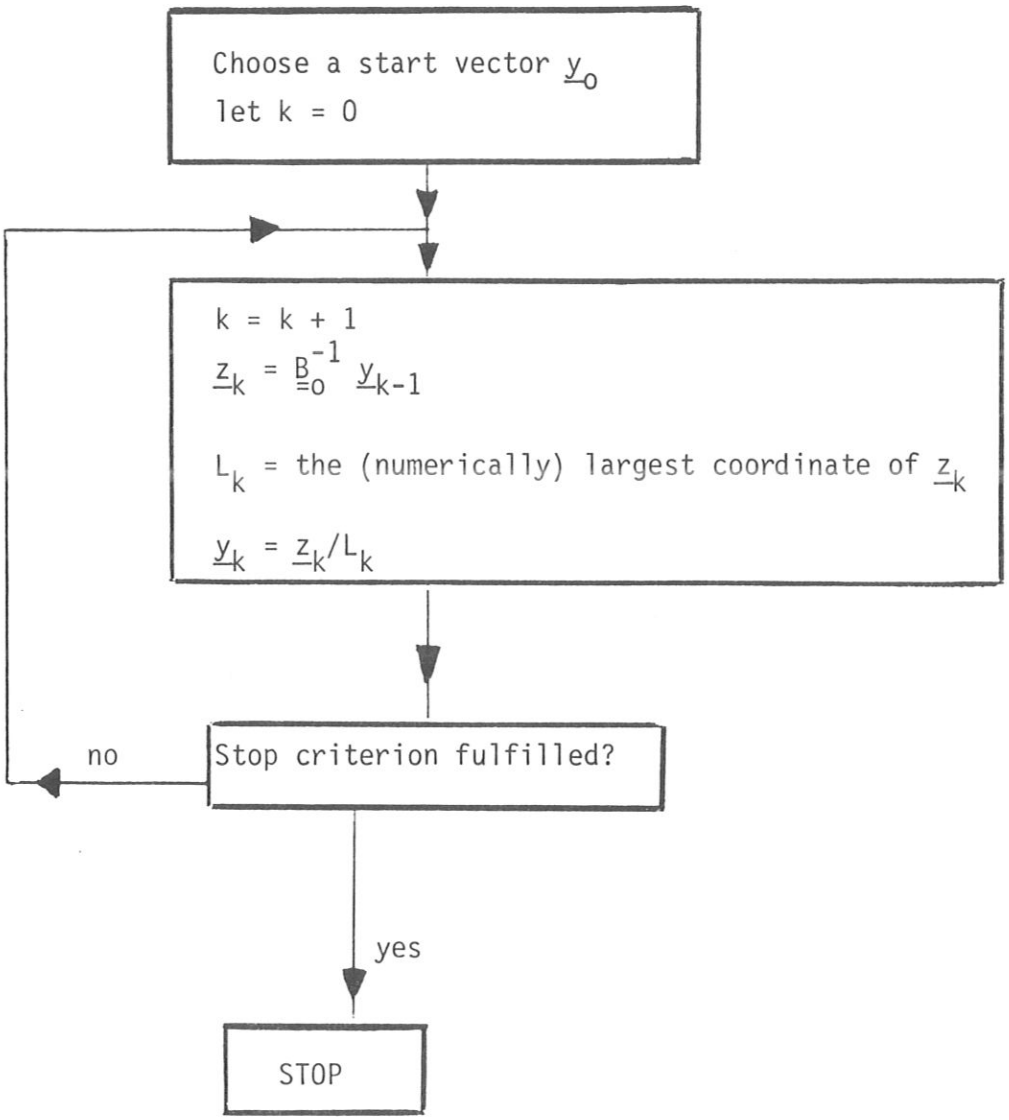
$$(Q_r - Q_o)^{-k} \{d_r \underline{s}_r + \sum_{l \neq r} d_l \left(\frac{Q_r - Q_o}{Q_l - Q_o}\right)^k \underline{s}_l\} \qquad (4.24)$$

From assumption b above $\frac{Q_r - Q_o}{Q_l - Q_o} < 1$, so

$$\underline{y}_k \rightarrow \frac{d_r}{(Q_r - Q_o)^k} \underline{s}_r \text{ , and } \frac{/\underline{y}_k/}{/\underline{y}_{k-1}/} \rightarrow \frac{1}{(Q_r - Q_o)} \text{ ,}$$

i.e. the iteration leads towards the direction of $\underline{s}_r$ and the value of Q_r. In order to avoid overflow, $\underline{y}_k$ is normalised in each step.

ii) Algorithm



We note that in this algorithm

$$\left.\begin{array}{l} L_k \to \dfrac{1}{Q_r - Q_o} \\ \underline{y}_k \to t \cdot \underline{s}_r \end{array}\right\} \quad \text{for } k \to \infty$$

where the value of the scalar t is unimportant, as we are only concerned with relative concentrations.

This means that we may also determine the 'true' eigenvalue Q_r from $Q_o + 1/L_k \to Q_r$ for $k \to \infty$.

iii) Practical calculation

In every step of the iteration process we calculate $\underline{z}_k = \underline{\underline{B}}_o^{-1} \underline{y}_{k-1}$ (see algorithm), or actually we solve the equation

$$\underline{\underline{B}}_o \underline{z}_k = \underline{y}_{k-1} \tag{4.25}$$

for $\underline{z}_k$. This is done by means of Gauss's elimination method (reducing $\underline{\underline{B}}_o$ to triangular form) and should really be accompanied by partial pivoting /19/. Fortunately experience has shown that pivoting is unimportant in our case, so that it is simple to 'remember' how the elimination procedure is performed.

'Remembering' the elimination procedure is useful, because $\underline{\underline{B}}_o$ is the same in every step of a given iteration, so that we may save time by reducing $\underline{\underline{B}}_o$ to triangular form once at the beginning of the iteration, and then only apply the procedure to $\underline{y}_{k-1}$ in the k'th step. Of course this could also be done including pivoting.

After thus rewriting eq. (4.25) we easily solve for $\underline{z}_k$ by back-substitution.

4.5 Optimizing program

The listed versions (Chapter 5) have not been optimized with respect to time and space requirements. This is so partly because of the size and speed of the Amdahl 470, partly because these versions were intended for several different users and a variety of applications.

Users with a narrower range of applications, or with a smaller computer, may however wish to optimize their version correspondingly. An example is described in Section 5.9. Actually we suggest, that one might design a version of SQUEAKIE to run on a small personal computer (!) by tailoring it closely to a particular type of application.

Quite generally one may save computertime by using a simpler analytical expression for the stopping power (Sect. 4.3). Using eq. 4.12, the stopping power calculations take almost 70 % of the CPU-time! In contrast, the expression 4.13 is more than 3 times as fast to calculate, both on the NORD-100 and on the Amdahl 470 —— on an ABC 80 personal computer it is $\sim$ 7 times as fast as eq. 4.12.

In as far as space requirements are concerned we note, that the listed versions use an excessive number, and size, of arrays. If necessary, most users could easily limit the interesting part of their spectrum to much less than 1024 channels. Also, one does only rarely consider signals from more than 4 elements at a time, when measuring depthdistributions (the present version allows up to 6 elements). Omitting the calculation of 'integrated contents' (Sect. 3.3) also saves you an array. Finally the present version allows up to 500 depthsteps, whereas $\sim$ 50 usually suffice.

Transferring all major arrays (particularly 'SPCT') to COMMON blocks is certain to save space, and the array 'DESCR' is specific for use in Garching. Also the use of double precision constants and variables is usually unnecessary.

For further discussion of program optimization the reader is referred to Sect. 5.9.

5. P R O G R A M

1. The versions listed and described most extensively below both reside on the Amdahl 470 at the Max-Planck-Institut für Plasmaphysik (IPP) in Garching. This computer is so large and fast that little effort was devoted to saving time or space in these versions (see Sect. 4.5).
   The necessary core storage is ∿ 110 K bytes, plus several K bytes for the operating system and buffers. Requesting space in portions of 60 K we occupy a total of 180 K, which is low enough to give the program a high priority in the job-queue.
   The total CPU-time varies faster than linearly with both the number of target elements, m_e, and the number of depthsteps, i.e. with the maximum depth evaluated. Typical CPU-times are ∿ 3 seconds for a target containing 4 elements evaluated in 30 depthsteps.

2. It may often be desirable to use the program on much smaller computers, so a version residing presently on the NORD-100 computer at the University of Aarhus is also briefly described. This version is somewhat more specific for the computer, so it is not listed here, but the optimization relative to the Garching-versions is discussed. Computing time was reduced as suggested in Sect. 4.5, so that the evaluation of a target containing 4 elements in 30 depthsteps typically takes ∿ 17 seconds.

3. The listed versions are specific for Rutherford Backscattering (RBS) spectra, but along with the description of the program, the few changes necessary for nuclear reaction energy spectra are indicated:

It is here assumed, that m_e possible targetelements are specified in the input (see below), and that the experimental spectrum is composed of RBS-signals from some of the m_e-1 first elements and nuclear reaction signals from element number m_e. Usually, though, the resolution is much poorer for the nuclear reaction signals than for RBS, so one should consider also the possible problems concerning the comparison of such quite differently smeared signals (see also Sect. 7.2).

4. The purpose of the following description is to enable users to understand existing versions of the program, or possibly implement new versions on their own computer. The latter is perhaps a rather optimistic aim, as experience proves it quite difficult to make the necessary modifications in a program written by somebody else. In an attempt to overcome this, the present program is not only listed, but also explained in extreme detail - almost down to every single statement. This should also be helpful to those who prefer to design their own (superior?) program.

   The statements of a given segment are identified by the numbers to the very left in the listing below.

   If you are implementing the listed code on your computer, Section 7.1 may help you to catch programming errors, etc.

5.1 - 5.8

These sections all reside separately on the Amdahl 470. Both listings and descriptions are continuously updated as the program is being improved during use. The latest version may at any time be requested from the authors.

5.9 Aarhus-version

As an example of an alternative version of SQUEAKIE, the version residing presently on the NORD-100 computer in Aarhus is briefly described and commented upon below. The NORD-100 is considerably smaller than the Amdahl 470. It is equipped with a 64 kbyte 16 bit memory, and a real constant or variable occupies 3 bytes (words).

After optimization with respect to time and space (see below) the program code takes up 20.7 kbytes and the COMMON blocks 19.3 kbytes of memory, so the program is easily hardled by the NORD-100 with respect to memory requirements. The optimized program has even been extended somewhat compared to the Garching versions.

A listing of the Aarhus-version may be requested from the authors at any time. In the following the reader is expected to be familiar with the descriptions of the IPP-versions (see previous sections).

i) Changes

Only minor modifications of the IPP-versions were absolutely necessary for making the program run on the NORD-100. These changes are nearly

all in the SQUEAKIE main program (compare Sect. 5.1) and concern the input/output statements.

Such a modified version, however, was found to be quite slow on the smaller computer. As discussed in Sects. 4.3 and 4.5 the CPU-time was considerably reduced by using instead the expression (4.13) for the stopping powers. The function STPA (Sect. 5.5) was therefore replaced by calls to existing subroutines /17/.

ii) Extensions

a) A preliminare subroutine has been included for the purpose of plotting the results. This is naturally a very machine dependent part of the program: The plotting is based on the two arrays (in subroutine STEP) 'CMP' and 'XINT', holding the calculated composition and the depth step lengths, respectively. These two arrays are moved to a common block for easier transfer to the plotting subroutine.

b) A new tool in the Aarhus version is the inclusion of limitations for each element: A lower and an upper channel number is specified for each element, defining the interval within which signals from this element may occur. This is a very useful feature, since the program may not always distinguish between signals from light elements at the surface or heavier elements at larger depths (see also Section 5.8).

In practice a statement has been included in STEP, checking in each depthstep whether the channel number considered for a given element lies within the specified interval. If this is not the case, the elemental signal from this depthstep is ignored.

The element limitations should be used with care only. They require a certain pre-knowledge of the target/spectrum, but in many cases such a knowledge is present or can be acquired by a visual inspection of the spectrum.

c) The specification of the element limits is done in a subroutine also used for subtracting background signals. This subroutine is used in connection with a standard, interactive fitting program on the NORD-100, and is written for the specific purpose of supplying a background subtracted spectrum as input to SQUEAKIE. The background is fitted separately for each elemental signal, and the limits of the interval, within which the background is actually subtracted, are used afterwards as the element limits mentioned above. The nature of such a background subtraction necessitates a certain experience and knowledge of both the fitting procedure and the nature of the spectrum.

iii) Optimization

The program was optimized in various ways relative to the IPP-versions (see also Sect. 4.5):

a) All major arrays were transferred to the common area. The program then takes up less space, when it is saved on disk, and the transfer of parameters to subroutines is made easier.

The IPP-versions use double precision constants and variables, but this has been found to be unnecessary and is changed to single precision in the Aarhus version. Besides from a small reduction in size, the program becomes 8 % faster, since some time consuming routines for converting from double to single precision are no longer needed.

b) Since the NORD-100 is considerably slower than the Amdahl 470 some efforts have been made to speed up the program execution. For this purpose the CPU time-consumption in the various parts of the program were analyzed using a standard CPU measurement facility in the NORD system. The analysis shows that nearly 90 % of the CPU-time is used in the 'DO 140'-loop (Sect. 5.7) of STEP, and especially in the herein nested 402 and 403-loops. The time here mainly goes to calculating the stopping powers. The use of a stopping power expression which is 3 times faster than the Ziegler expression used in Garching (Sect. 4.3), made the whole program about 2.3 times faster.

The CPU-time was further reduced by 8 % by doing some calculations once instead of 3 times, again in the 402 and 403-loops: In these statements the appropriate parts (CMP(NE,NI) * 1.E-15 and XINT(NI)/CBET*1.E-3) are replaced by variables, which are calculated only once for each pass through the loop.

c) After the above optimizations a typical CPU-time measurement shows the following distribution of time consumption:

subroutine STEP		17 %
subroutines ITER, CRSEC, XK	total	1 %
subroutine STOPP (the stopping power expression)		44 %
subroutine HELI4 (selects the 3 constants for STOPP)		6 %
various system and FORTRAN routines for transfer of parameters, subroutine calls, etc.		32 %

Actually, in the calculation of the stopping power a certain time is also needed for parameter transfer etc., so that in the final program nearly 70 % of the CPU-time is devoted to stopping power calculations.

The total CPU-time for a given job is highly dependent on the number of elements, m_e, and the number of steps into the target, m_s. In the time consuming 'DO 140'-loop (see above) the total number of calls to subroutine STOPP is found to be

$$m_e^2 \cdot 3 \frac{(m_s-1)\,(m_s-2)}{2} + m_e$$

which is roughly proportional to $m_e^2 \cdot m_s^2$. This is in fine agreement with the empirical finding, that the total CPU-time is proportional to $(m_e \cdot m_s)^{1.7}$.

iv) Example

For an illustration of the use of the Aarhus-version a simple RBS-spectrum (Fig. 3a) is chosen. This is a spectrum of an Al-Co-Au alloy which has been prepared by a vacuum co-evaporation of the 3 elements on a carbon substrate. It is normally used for energy calibration because the 3 elements (all present at the surface) yield 3 distinct high-energy edges in the spectrum. A closer inspection of the low-energy signals (Fig. 3b) shows that a little native oxide was present on the carbon substrate before evaporation. Furthermore one finds carbon and oxygen as contaminants on top of the alloy, and since these signals only appear after months of use they are ascribed to respectively cracking of diffusion pump oil and oxidation of the sample.

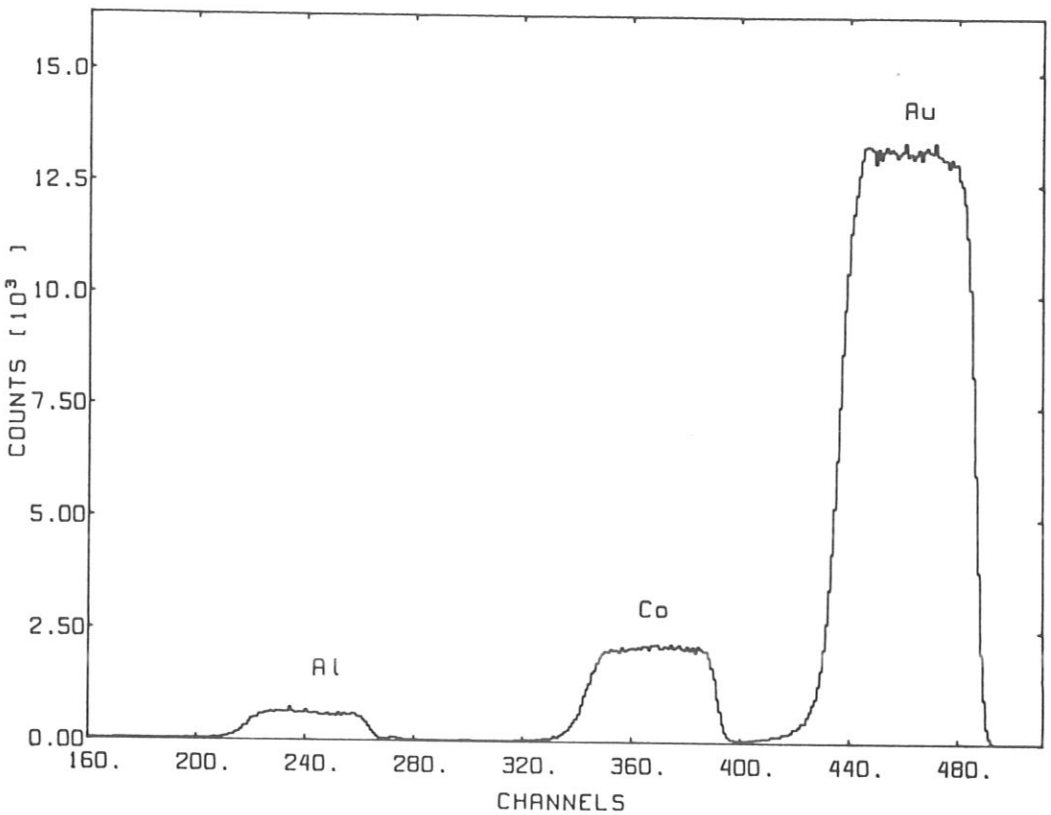


Fig. 3a: RBS-spectrum of Al-Co-Au alloy on a carbon substrate. High-energy signals

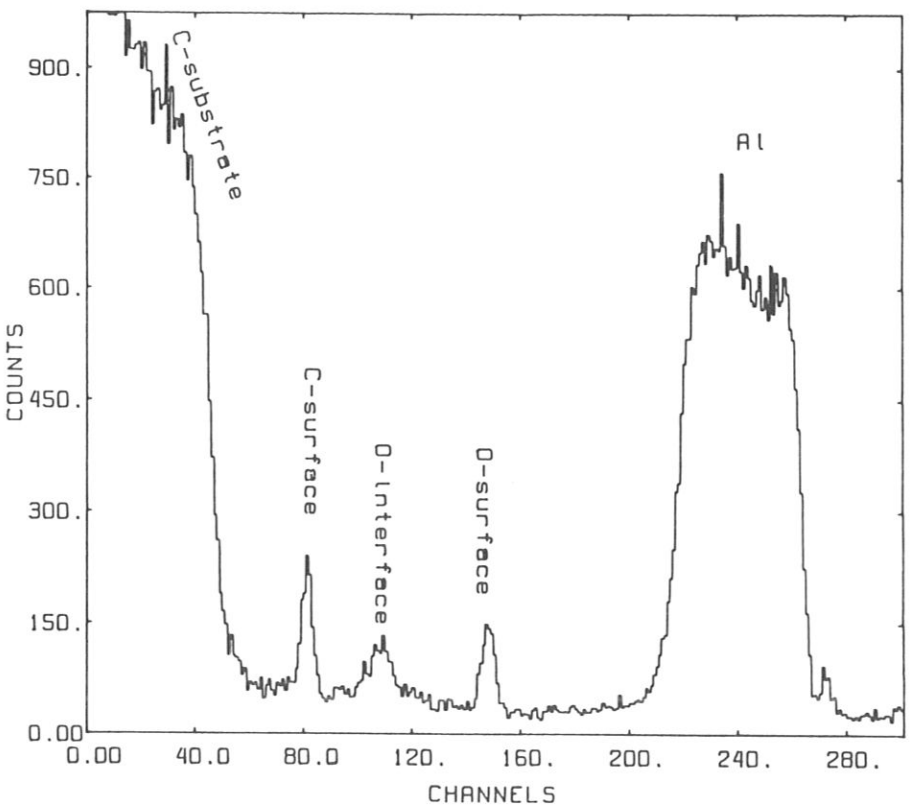


Fig. 3b: Low-energy signals (note change of scale)

The need for both background subtraction and element limits, as discussed above, is clearly seen in Fig. 3b. (In Garching background subtraction must be performed by an independent program.) The background was here fitted by a straight line through channels 88-96 and 157-165 (see Fig. 3c), and then subtracted in the whole region between the channels 88 and 165 to yield the oxygen signals. The channels 88 and 165 are then used as 'element limits' for oxygen.

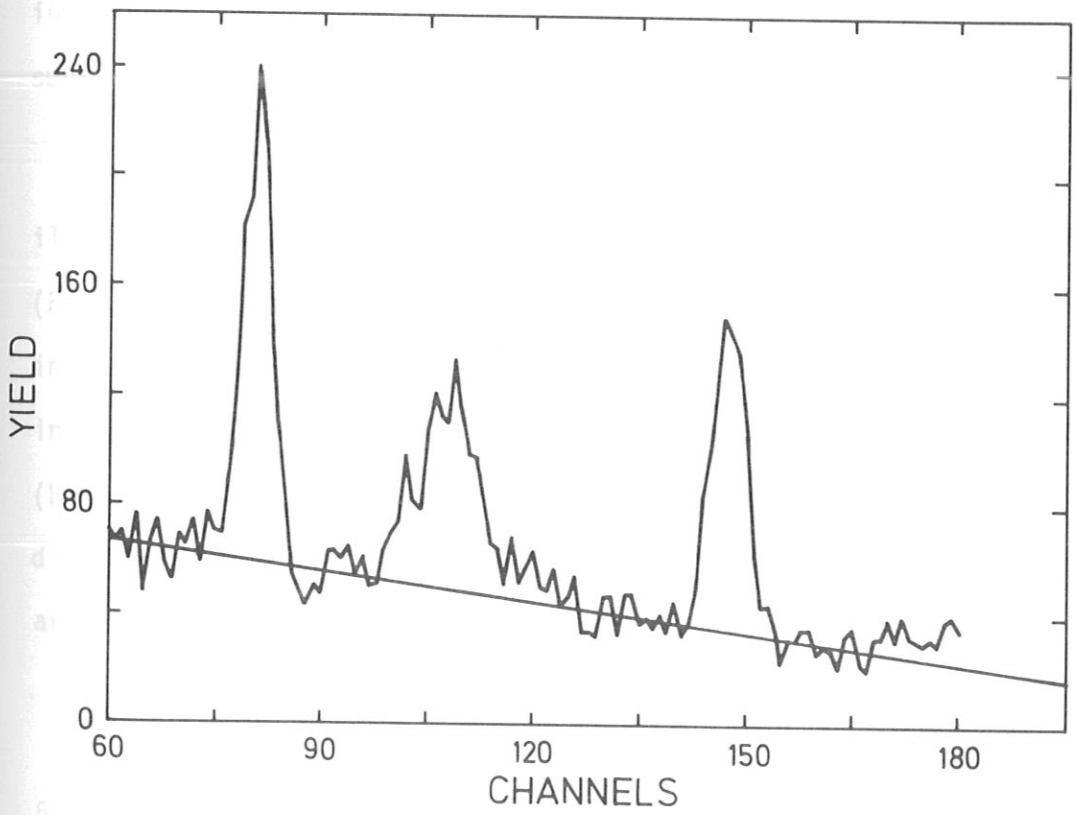


Fig. 3c: Part of spectrum expanded: Signals from C at the surface, and O at surface and interface. Straight line —— background to be subtracted from signals

After all the elemental signals have been corrected for background and supplied with element limits, a run of SQUEAKIE yields the results of Fig. 4a. The depth distribution shows the expected thin layer of carbon and oxygen on the surface of a nearly homogeneous Al-Co-Au alloy. The Q-value ($N_{prim}\Delta\Omega$, Sect. 2.2) is estimated in each step, and for the present case it is plotted as a function of depth in Fig. 4b.

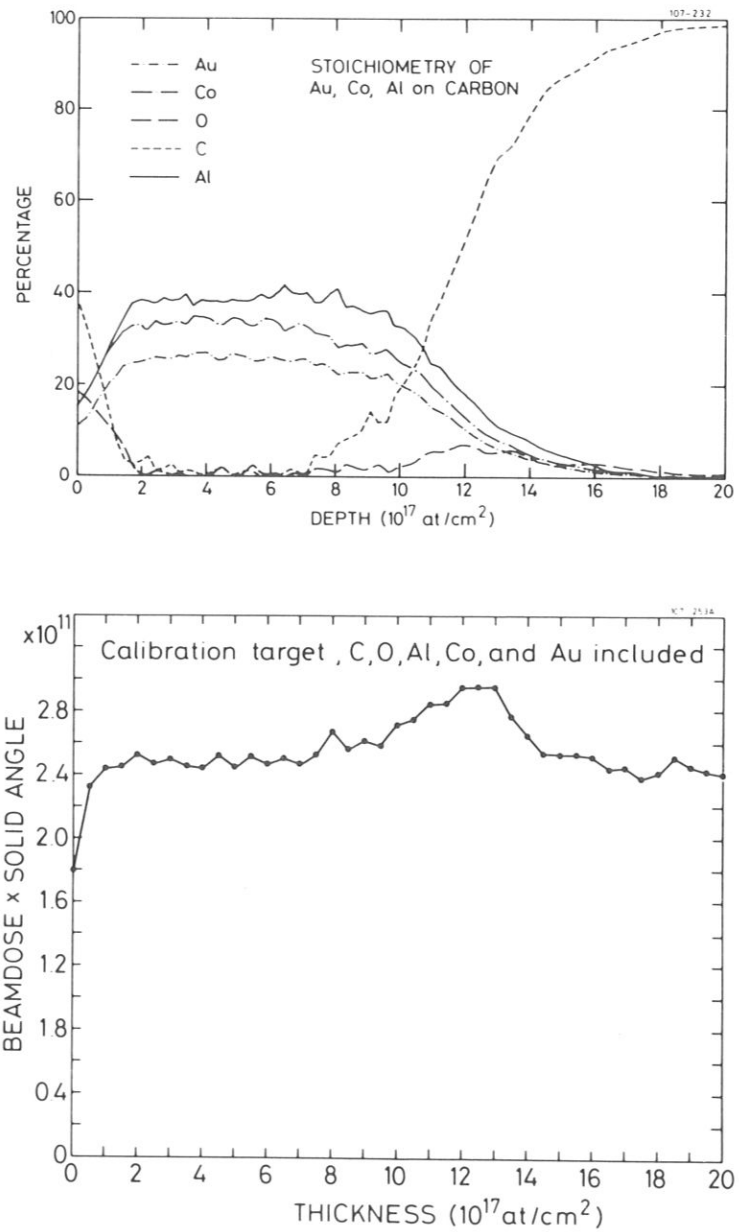


Fig. 4: Results obtained from spectrum in Fig. 3 by means of SQUEAKIE
a) Relative elemental concentrations vs. depth
b) Eigenvalue Q vs. depth. Note different depth scales!

This value can in a way be taken as a measure of the validity of the calculations:

The Q-value is actually a physical constant for a given spectrum, so for a correct calculation it should remain independent of depth. This argument, however, is somewhat obstructed by the possibility of 'cancellation of errors' /1/, where a correct stoichiometry may result from the relative signal heights while the absolute error is absorbed in Q. In Fig. 4b the Q-value is constant ($2.5 \cdot 10^{11}$) except at the surface and at the interface, where resolution effects, and possibly insufficient background subtraction, obscure the signals.

The behaviour of Q vs. depth in the case of errors is further illustrated by an alternative SQUEAKIE calculation on the same spectrum (Fig. 5). This time the carbon and oxygen signals are ignored, resulting in somewhat different results at larger depths (no signals), as seen in Fig. 5a. This "lack of signal" is reflected in the low Q-values (Fig. 5b), especially beyond $1.2 \cdot 10^{18}$ atoms/cm^2, where the depth distribution becomes clearly unrealistic. However, the elemental ratios are nicely reproduced at those depths, where Q remains constant.

5.10 List of symbols

Unfortunately it has not always been practical to use the same symbol for a variable or constant in the program and in the present text. The following list should help avoid confusion.

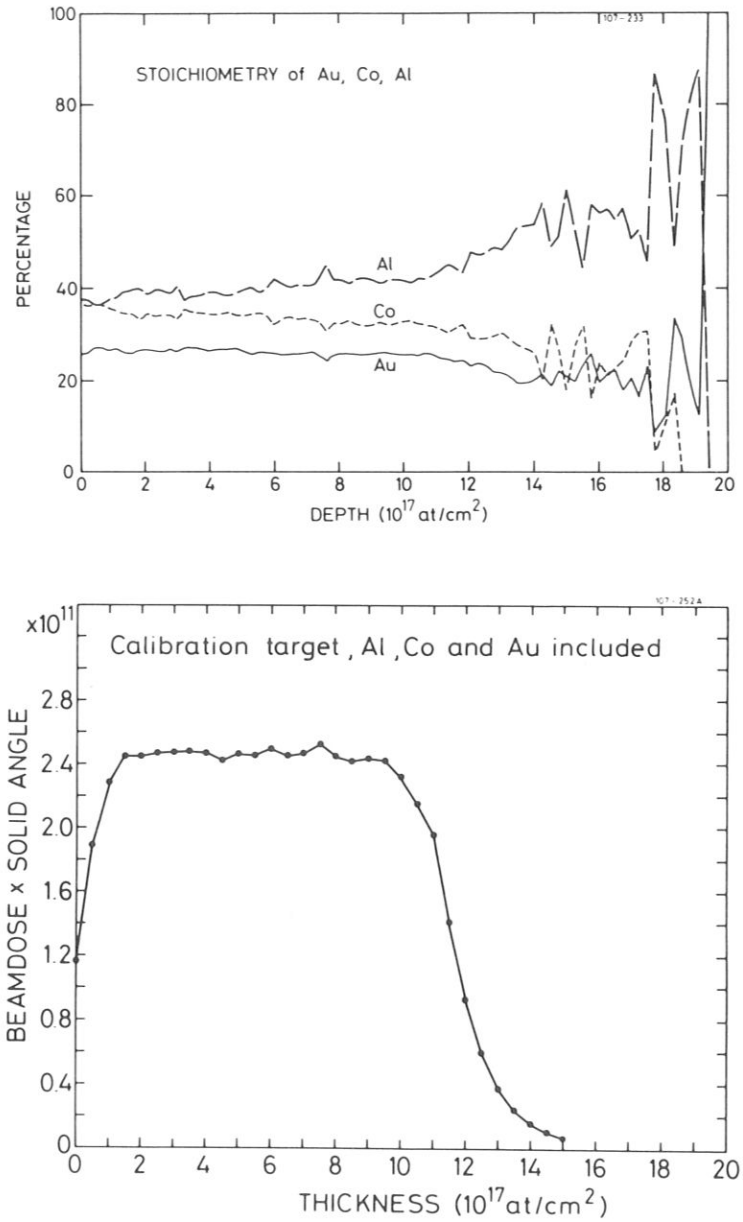


Fig. 5: As Fig. 4, but ignoring signals from C and O.

Text	Program	Meaning
m_e	NTOT	Total number of elements possibly present in target
m	N	Dimension of $\underline{\underline{D}}$ at given depth = number of elements at this depth
Q_o	QØ	Initial 'guess' of eigenvalue at given depth
$\underline{\underline{D}}$	AM	Matrix $\underline{\underline{D}}$ of eigenvector problem (eq. 2.12)
$C_i a_{ij}$		element of $\underline{\underline{D}}$
Q_r		True eigenvalue at given depth (the one we want)
$\underline{s}_r$		True eigenvector at given depth (the one we want)
$\underline{s}_j$		Some true eigenvector at given depth (not necessarily the one we want)
$\underline{\underline{B}}$		$= \underline{\underline{D}} - Q_m \underline{\underline{I}}$
$\underline{\underline{B}}_o$	A (in ITER)	$= \underline{\underline{D}} - Q_o \underline{\underline{I}}$
M_i	A (in XK, STPA)	Masses of target elements
b^o_{ij}		element of $\underline{\underline{B}}_o$
M_1	A1	projectile mass
E_o	EØ	primary beam energy at target surface
α	ALFA	incident angle
n_i		relative atomic concentration of element 'i' at depth x

x	X	depth below target surface
S^i_{pj}		stopping power for particle 'pj' in targetelement 'i'
S^i		stopping power for projectile in targetelement 'i' (RBS-exp.)
Z_1	IZ1	projectile atomic number
ch1(i)	IH1(i)	lowest channel in signal from 'i'
ch2(i)	IH2(i)	highest channel in signal from 'i'

6. HOW TO USE THE PROGRAM

Below is described how to run the 2 existing versions of SQUEAKIE on the Amdahl 470 in Garching.

The first "problem" is to choose the appropriate version. This is best done by studying Sect. 6.5: For most purposes the alternative version (submitted as "SQU", Sect. 6.1) is the simpler one to use.

Section 6.1 demonstrates how to submit both versions for execution. This is followed by a short note (Sect. 6.2) on the job control cards. Note that these differ, depending on whether or not results from a previous run are included (see also Sect. 3.4).

The necessary input, and its format, is then described (Sect. 6.3), followed by an explanation of the output expected on various output-devices (Sect. 6.4).

The last two sections may also be of some interest for users elsewhere: A few examples of input and output are given in order to illustrate the preceding sections. Finally follows an assortment of warnings which may prove vital to any user.

Note: In case the system is changed, corrections to this Chapter will be listed together with Sections 5.1 - 5.8 on the Amdahl 470.

6.1 Submit

a) The original version (Sects.5.1-5.7) employs the stop-criteria described in Section 3.4.
This version is chosen by submitting the AMOS-segment PRB: A.SQ.
The necessary modifications of this segment are described in the following section.
For most applications the program may be submitted with the command XS PRB: A.SQ.

b) The alternative version (Sect. 5.8) employs elemental 'markers' instead of the stop-criteria of Section 3.4.
This version is chosen by submitting PRB: A.SQU, usually with XS.

c) For frequent use, please create your own control cards, input- and output-segments.

6.2 Job control cards

On the Amdahl 470 the program is preceded by a set of job control cards. This also links the various segments of the program (Sects. 5.1-5.6) together. Output is routed to the remote station RMT 10 (PWW).

a) Two examples of the use of the original version (SQ) are shown below, one for the case where previous runs are ignored, one for the case where results of a previous run are included. The input parameters (Sect.6.3) are found on the segment PRB:C.EUSDT.

1. example: This is the most common situation. The experimental spectrum is found on the segment BOM:BMSD4.SEG57. The output segment is PRB:B.EUS55.

No previous runs are included.

```
/*ROUTE  PRINT RMT1Ø
/*JOBPARM SYSAFF=S87Ø
//*       PRB:A.SQUEAKIE
// EXEC FORTRAN
//C.SYSPRINT DD SYSOUT=Z
//C.SYSIN DD *
$$ PRB:A.SQUEAKIE
$$ PRB:A.CRSEC
$$ PRB:A.XK
$$ PRB:A.STPA
$$ PRB:A.STEP
$$ PRB:A.ITER
//G.SYSLOUT DD DUMMY
//G.FT31FØØ1  DD DSN='AMOS-PRB:B.EUS55,W',
$$                SYS:DD.F8Ø
//G.SYSIN DD *
$$ PRB:C.EUSDT
$$ BOM:BMSD4.SEG57
```

2. example: As mentioned in Section 3.4 and illustrated in Section 6.5 one may wish to include the results of a previous run. In example 1 (above) the results were tabulated on the segment PRB:B.EUS55. If we now want to include these results in an evaluation of the spectrum BOM:BMSD4.SEG55 obtained from the same target, we modify the job control cards as follows:

The segment PRB:B.EUS55 is linked to the data in the input stream, and a new output segment (PRB:B.EU355) is specified.

```
/*ROUTE  PRINT RMT1Ø
/*JOBPARM SYSAFF=S87Ø
//*       PRB:A.SQUEAKIE
// EXEC FORTRAN
//C.SYSPRINT DD SYSOUT=Z
//C.SYSIN DD *
$$ PRB:A.SQUEAKIE
$$ PRB:A.CRSEC
$$ PRB:A.XK
$$ PRB:A.STPA
$$ PRB:A.STEP
$$ PRB:A.ITER
//G.SYSLOUT DD DUMMY
//G.FT31FØØ1  DD DSN='AMOS-PRB:B.EU355,W',
$$                SYS:DD.F8Ø
//G.SYSIN DD *
$$ PRB:C.EUSDT
$$ BOM:BMSD4.SEG55
$$ PRB:B.EUS55
```

b) For the alternative version the job control cards are identical, except for replacing the segments A.SQUEAKIE and A.STEP by the segment A.ALTER.

This is actually only a formal replacement, as the latter segment uses both the others. Both A.SQUEAKIE and A.STEP must therefore also exist, when the alternative version is used.

```
/*ROUTE  PRINT RMT1Ø
/*JOBPARM SYSAFF=S87Ø
//*       PRB:A.SQUEAKIE
// EXEC FORTRAN
//C.SYSPRINT DD SYSOUT=Z
//C.SYSIN DD *
$$ PRB:A.ALTER
$$ PRB:A.CRSEC
$$ PRB:A.XK
$$ PRB:A.STPA
$$ PRB:A.ITER
//G.SYSLOUT DD DUMMY
//G.FT31FØØ1  DD DSN='AMOS-PRB:B.EU355,W',
$$                SYS:DD.F8Ø
//G.SYSIN DD *
$$ PRB:C.EUSDT
$$ BOM:BMSD4.SEG57
```

6.3 Input

a) Original version (Sects. 5.1-5.7), "SQ".

The amount of input parameters and data depends somewhat on the problem, but the first set of records is always needed:

Record # 1

Columns 1- 7 (F7.1): Scattering angle θ, in degrees.

" 11-17 (F7.1): Incident angle α, in degrees.

" 21-27 (F7.1): Detector angle ß, in degrees.

Record # 2

Columns 1- 7 (F7.Ø): Incident energy E_0, in keV

" 11-18 (F8.3): Energy per channel ΔE_1, in the spectrum, in keV

" 21-28 (F8.3): Energy offset in calibration (energy of channel no. Ø), in keV

Record # 3

Columns 1- 7 (F7.Ø): Minimum inward beamenergy E(x) of interest (determines max. depth x), in keV

" 11-13 (I3): Lowest channelnumber of interest

" 17 (I1): Flag. Integrated contents vs. depth tabulated for flag > Ø.

" 19 (I1): FWHM of the exp. resolution at the surface (only used for integrating contents), in number of channels

" 21 (I1): Flag. Targetcomposition derived previously is read in, if flag > Ø. In that case only one experimental spectrum is allowed (see Record # 5).

Record # 4

Columns 1-2 (I2): Number m_e of possible target elements to look for.

Record # 5

Columns 1-2 (I2): Number of experimental spectra to be evaluated with this set of input parameters (see Record # 3, Col. 21)

" 6-9 (I4): Number of points in each experimental spectrum.

Record # 6

Columns 1-1Ø (F1Ø.3): The projectile mass M_1, in a.m.u.

" 16-17 (I2): The atomic number Z_1 of the projectile

" 21-3Ø (F1Ø.3): The energy-scaling factor "FE" used in the function "STPA" for calculating the stopping power of isotopes. Equals 1.Ø for ^{4}He and ^{1}H.

The following datapack must contain 2 records for each of the m_e targetelements (see Record # 4 above). The first record specifies the element, the second the corresponding stopping power coefficients:

Record # 7

Columns 1-1Ø (F1Ø.3): The mass M_i of the first element, in a.m.u.

" 15-17 (I3): The atomic number Z_i

" 2Ø-21 (A2): The chemical name of the element.

Record # 8, for use of He-projectiles

Columns	1-13 (E13.4):	Stopping coefficient A1 /11/
"	15-27 (E13.4):	" A2 /11/
"	29-41 (E13.4):	" A3 /11/
"	43-55 (E13.4):	" A4 /11/
"	57-69 (E13.4):	" A5 /11/

for the first element.

Record # 8, for use of H-projectiles

Columns	1-13 (E13.4):	Stopping coefficient A2 /12/
"	15-27 (E13.4):	The number Ø.45 DØ
"	29-41 (E13.4):	Stopping coefficient A3 /12/
"	43-55 (E13.4):	" A4 /12/
"	57-69 (E13.4):	" A5 /12/

Record # 9

Columns	1-1Ø (F1Ø.3):	The mass M_i of the second element, in a.m.u.
"	15-17 (I3):	
	and so forth ---	

The final datapack must now contain one or two sets of data for each experimental spectrum (Rec. # 5, Cols. 1-2), depending on the flag in Col. 21 of Rec. # 3.

In any case the pack must of course include the experimental spectrum, on the form automatically created in AMOS:

i. The spectrum is preceded by a 'descriptor' - 10 lines (records) containing optional alphanumeric text in columns 1-72. This is printed again on all output for identification.

ii. This is followed by a listing of the spectrum itself, 10 channels per line (record) in the columns 1-7, 8-14, 15-21, 22-28, 29-35, 36-42, 43-49, 50-56, 57-63, and 64-70. Format F 7.Ø.

If more data are to follow, it is essential that the number of points in the spectrum were correctly given in columns 6-9 of Record # 5. This is for instance the case if the flag in column 21 of Record # 3 was positive. In that case the present datapack must also include a table listing target composition vs. depth, with the elements in the same order as in the datapack above:

iii. Also this table is preceded by a 10 line descriptor, on the same form as for the spectra. This is not printed on output!

iv. The table itself consists of an optional number of lines, each giving in

Columns	11-2Ø (E1Ø.3):	The depth x, in atoms/cm^2
"	26-3Ø (F5.3):	The relative concentration n_1 of the first element
"	34-38 (F5.3):	The relative concentration n_2 of the second element
"	42-46 (F5.3):	n_3
"	50-54 (F5.3):	n_4
"	58-62 (F5.3):	n_5
"	66-70 (F5.3):	n_6

We note that this table is on the same form as the output to be printed on a data file (below). We may thus directly use the output from a previous run of the program.

b) Alternative version (Sect. 5.8), "SQU".

The input parameters are almost the same as for the original version:

Record # 1

Columns	1- 7 (F7.1):	Scattering angle θ, in degrees.
"	11-17 (F7.1):	Incident angle α, in degrees
"	21-27 (F7.1):	Detector angle ß, in degrees

Record # 2

Columns	1- 7 (F7.Ø):	Incident energy E_0, in keV
"	11-18 (F8.3):	Energy per channel ΔE_1 in the spectrum, in keV
"	21-28 (F8.3):	Energy offset in calibration (energy of channel no. Ø), in keV

Record # 3

Column 17 (I1): Flag. Integrated contents vs depth tabulated for flag > Ø.

" 19 (I1): FWHM of the exp. resolution at the surface, in number of channels

" 21 (I1): Flag. Targetcomposition derived previously is read in, if flag > Ø.

Record # 4

Columns 1-2 (I2): Number m_e of possible target elements to look for.

Record # 5

Columns 1-2 (I2): Number of experimental spectra to be evaluated with this set of input parameters. (Must equal 1 if flag > Ø in Record # 3, Col. 21).

" 6-9 (I4): Number of points in each experimental spectru

Record # 6

Columns 1 -1Ø (F1Ø.3): The projectile mass M_1, in a.m.u.

" 16-17 (I2): The atomic number Z_1 of the projectile

" 21-3Ø (F1Ø.3): The energy-scaling factor "FE" used in the function "STPA" for calculating the stopping power of isotopes. Equals 1.Ø for ^{4}He and ^{1}H, 4/3 for ^{3}He and 0.5 for deuterons.

The following datapack must contain 2 records for each of the m_e target-elements (see Record # 4 above). The first record specifies the element, and the element limits, the second the corresponding stopping power coefficients:

Record # 7

Columns 1-1Ø (F1Ø.3): The mass M_i of the first element, in a.m.u.

" 15-17 (I3): The atomic number Z_i

" 2Ø-21 (A2): The chemical name of the element

" 3Ø-33 (I4): The lowest channel in which to find signals from this element.

" 4Ø-43 (I4): The highest channel in which to find signals from this element.

Signals from this element will be set equal to Ø if they do not fall between these limits.

Record # 8, for use of He-projectiles

Columns 1-13 (E13.4): Stopping coefficient A1 /11/

" 15-27 (E13.4): " A2 /11/

" 29-41 (E13.4): " A3 /11/

" 43-55 (E13.4): " A4 /11/

" 57-69 (E13.4): " A5 /11/

for the first element.

Record # 8, for use of H-projectiles

Columns 1-13 (E13.4): Stopping coefficient A2 /12/

" 15-27 (E13.4): The number Ø.45 DØ

" 29-41 (E13.4): Stopping coefficient A3 /12/

" 43-55 (E13.4): " A4 /12/

" 57-69 (E13.4): " A5 /12/

Record # 9

Columns 1-1Ø (1Ø.3): The mass M_i of the second element, in a.m.u.

" 15-17 (I3): The atomic ....

and so forth (as Record # 7) ...

If the flag in Rec. # 3, Column 21 equals Ø, the final datapack contains the experimental spectra on the form automatically created in AMOS:

i. The spectrum is preceded by a 'descriptor' - 10 lines (records) containing optional alphanumeric text in columns 1-72. This is printed again on all output for identification.

ii. The spectrum itself is listed with 10 channels per line (record), in the columns 1-7, 8-14, 15-21, 22-28, 29-35, 36-42, 43-49, 50-56, 57-63, and 64-70. Format F7.Ø.

If the flag in Rec. # 3, Column 21 is positive, only one experimental spectrum is allowed. This is given on the form above, and followed by a table listing targetcomposition vs. depth:

iii. Also this table is preceded by a 10 line descriptor, on the same form as for the spectra. This is <u>not</u> printed on the output.

iv. The table itself consists of an optional number of lines (records), each giving in

Columns 11-20 (E1Ø.3): The depth x, in atoms/cm^2.

" 26-30 (F5.3): The relative concentration n_1 of the first element.

" 34-38 (F5.3): The relative concentration n_2 of the second element.

" 42-46 (F5.3): n_3

" 50-54 (F5.3): n_4

" 58-62 (F5.3): n_5

" 66-70 (F5.3): n_6

This table is on the same form as the output printed on a datafile (Sect. 6.4). We may thus directly use the output from a previous run of the program.

6.4 Output

Output is partly printed, partly listed on an output segment specified in the control cards (see Sect. 6.2).

Printed output

The output begins with a list of the input parameters used (compare previous section):

Scattering angle (θ), incident angle (α), and exit-angle (β), as read in from Record # 1.

Incident energy (E_0), energy per channel (ΔE_1), and energy of channel no. Ø, as read in from Record # 2. Minimum inward energy below which to stop evaluation, and lowest channelnumber, as read in from Record # 3. Number of spectra to be evaluated with this input, as read in from Record # 5.

Projectile mass (M_1) and atomic number (Z_1), as read in from Record # 6.

The energy-scaling factor (FE), as read in from Record # 6.

For each of the m_e possible targetelements then the chemical name, the mass (M_i), the atomic number (Z_i), and the 5 stopping coefficients.

After the inputparameters follows a listing of the experimental spectra, for later control and identification.

Finally, after each spectrum follows the calculated target-composition vs. depth:

Tabulated are the relative stoichiometric coefficients vs. depth. The depth is in units of atoms/cm^2, and the coefficients normalized so that the sum over all m_e elements equals unity. Along with each coefficient is given the statistical uncertainty as estimated from eq. 2.3.

Furthermore the table shows the approximate channels in which the elemental signals from each depth are found (the channelnumbers are listed in the format F5.Ø, i.e. the actual numbers used usually deviate from these with fractions of a channel).

Finally the table includes the improved eigenvalue Q calculated in each depthstep (Sect. 4.4). This value should be compared to the product $N_{prim}\Delta\Omega$ of beamdose and detector solid angle, if this is known. Variations in Q may indicate resolution effects or direct errors /1, 9/, but the interpretation is not always obvious. Thus large variations in Q near the surface frequently indicate a partial 'cancellation of errors' (see Section 7.2 and Ref. 1).

Following the calculated target composition vs. depth the output may include a tabulation of integral contents vs. depth. As described in Sect. 3.3 the integral content of an element may be calculated in two independent ways. Correspondingly, the table consists of two parallel lists of results:

1. The total number of atoms/cm^2 of an element found between the surface and the depth x may be directly calculated from the targetcomposition vs. depth listed above (Eq. 3.1). The results are thus based on relative scattering yields and the energy losses of the projectile, and are listed under the heading "FROM ENERGYLOSS". This approach is best for reasonably large depths x.

2. The total number of atoms/cm^2 of an element in a target may be independently calculated from the total scattering yield (Eq. 3.2). This approach is best for thin layers. Relating the numbers to a

depthscale of course implicitly involves the knowledge of the targetcomposition, but for many applications such a relation is really unnecessary. Listed are the integral contents times beamdose N_{prim} times detector solid angle $\Delta\Omega$ (Eq. 3.3). One obtains the total content of an element in number of atoms/cm^2 by dividing the listed quantity by $N_{prim}\ \Delta\Omega$ (taken from the table above, or determined independently).

6.5 Examples

Below are shown a few examples of use of the program. The program itself has no facilities to plot spectra or output, but we include figures here for the sake of illustration. The first examples are for the original version ("SQ"), the last example for the alternative version ("SQU").

1. The first example demonstrates the simplest application of the program:

   It was attempted to produce an EuS-film (constant stoichiometry) of thickness 1110 Å on a Si-substrate. Ion beam spectrometry only yields filmthicknesses in terms of areal densities (e.g. atoms/cm^2), but assuming 'bulk density' of the film the nominal value should be $\sim 2.1 \cdot 10^{17}$ EuS/cm^2.

   A Rutherford backscattering spectrum was obtained using 2 MeV $^4He^+$-ions and a scattering angle $\theta = 170^o$ (see Fig. 6). The target was tilted an angle $\alpha = 60^o$ in order to improve the depth resolution, resulting in a detectorangle $\beta = 60.5^o$. The energy calibration used was

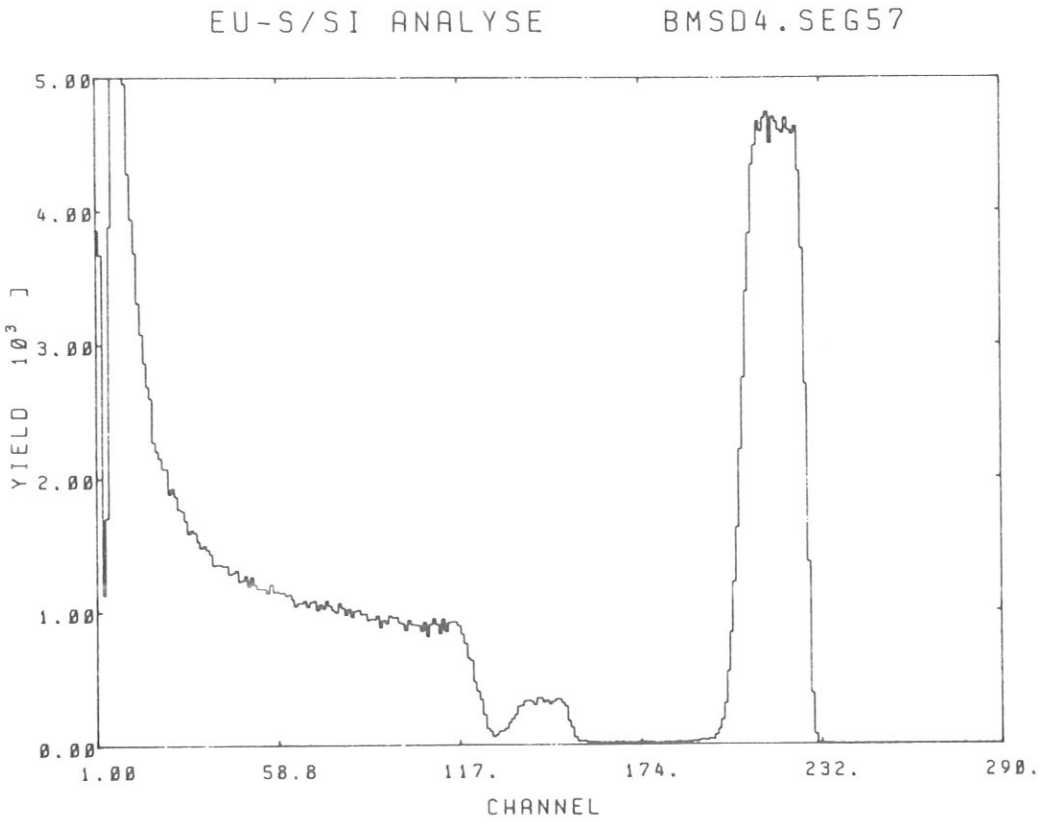


Fig. 6: RBS-spectrum of 2 MeV $^4He^+$-ions scattered from 1110 Å EuS on Si. $\theta = 170^\circ$, $\alpha = 60^\circ$, $\beta = 60.5^\circ$.

$$E_{det} = ch \times 7.683 + 55.0$$

where 'ch' is the channelnumber, and E_{det} is the corresponding energy in keV.

Of primary concern was the ratio of Eu- to S-contents in the film, so only these two elements were considered. For a beginning we make sure to evaluate the spectrum to sufficient depths - until the S-signal falls in a channel below 125. The necessary input was:

```
17Ø.Ø      6Ø.Ø       6Ø.5
2ØØØ.      7.683Ø     +55.ØØØ
15ØØ.Ø     125    1 2 1
 2
 1     289
4.ØØ16            2    1.Ø
32.Ø6              16    %
1.4Ø2       E+Ø 6.791       E-1 5.898       E+1 3.528       E+Ø 3.211       E+Ø
152.Ø             63    EU
1.4Ø2       E+1 3.63        E-1 2.284       E+2 7.Ø24       E+Ø 1.Ø16       E+Ø

   29Ø   44Ø1   469Ø   11Ø4   68ØØ      Ø       Ø       Ø       1
AMOS-FI-SG: BMSD4.SEG57          EXPERIMENT: EU-S/SI ANALYSE
NAME.....: BOR/SCHE              DATE/TIME.: 27: 7:82 / 16:28:21
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 6ØDEG
ANAL.DOSE.: 1.25E-7 C            ANAL.ENERG: 2 MEV
THETA.....: 17Ø DEG              MATERIAL..: 111Ø A EUS/SI
TARGETPOS.: 29 MM                LOGBOOK...: BMS II/23
NOTE1.....: 5ØØ CH./1Ø V         NOTE2.....: HV 256X
  3859   3673   1138   1788   3891   6Ø28   6888   6354   5533   4955
  4261   3937   3685   3311   3Ø77   2865   2685   2597   2273   22Ø3
  2151   2Ø7Ø   2Ø72   1881   1927   1863   1767   1755   1679   1584
  1615   1594   1525   1475   1499   1464   143Ø   1345   1354   1354
  1343   1344   128Ø   1293   131Ø   1224   1235   127Ø   1191   1261
  1233   1171   1171   1177   1142   12Ø5   1146   1156   1142   1146
  1118   1131   1Ø95   1Ø43   1Ø68   1Ø68   1Ø84   1Ø37   1Ø77   1Ø84
  1Ø12   1Ø6Ø   1Ø25   1Ø83   1Ø44   1Ø11    992   1Ø69   1Ø29    976
  1Ø22    959   1Ø85   1Ø16    981    986    932    945    94Ø    97Ø
   879    939    91Ø    97Ø    956    959    916    9Ø5    86Ø    939
   9ØØ    897    894    849    921    812    9Ø7    949    9Ø4    831
   947    848    92Ø    923    926    894    827    759    652    634
   47Ø    4ØØ    34Ø    228    125    1ØØ     64     81    1Ø6    112
   128    173    2Ø2    231    295    297    331    338    33Ø    3Ø3
   356    355    321    336    3Ø5    33Ø    346    347    314    289
   182    134     59     28     28     34     24     21     22     21
    15     21     15     18     13     24     15     22     13     19
    14     17     19     17     23     2Ø     21     17     13     15
    16     21     21     17     19     26     19     18     19     29
    28     3Ø     35     41     32     44     42     76    121    188
   3Ø9    55Ø    842   1219   163Ø   2216   2749   3398   3Ø32   4348
  4495   4676   4598   4699   474Ø   45Ø5   47Ø7   4668   46Ø6   4586
  4696   46Ø5   4577   4636   4299   3715   2698   1364    379     77
     8      8      4      7      6      Ø      2      5      2      3
     4      1      5      3      1      5      2      2      1      1
     2      Ø      1      Ø      2      3      Ø      1      3      3
     Ø      1      3      1      3      2      4      2      Ø      1
     1      2      Ø      1      1      2      2      1      Ø      1
     2      2      Ø      2      1      1      1      Ø      Ø      1
```

On the output we find first a list of the input used, for control purposes and identification. Then follows a table of the stoichiometric coefficients vs. depth. Along with each coefficient is given the estimated statistical uncertainty, and furthermore are listed the corresponding channelnumbers in the experimental spectrum. Also included in the table are the improved estimates of the eigenvalue Q (Section 4.4). Finally is printed a table of 'integrated contents' vs. depth.

SCATTERING ANGLE = 170.0 , INC.ANGLE = 60.0 AND EXIT-ANGLE = 60.5 DEGREES

INCIDENT ENERGY = 2000. KEV, 7.683 KEV/CHANNEL, AND ENERGY = 55.000 IN CHANNEL 0

STOP EVALUATION WHEN EBEAM< 1500. KEV, OR WHEN CHANNELS BELOW CH. 125 ARE REQUESTED

1 SPECTRA ARE EVALUATED WITH THIS INPUT

PROJECTILE HAS MASS = 4.002, AND Z = 2
ENERGY-SCALING FACTOR 1.020

TARGET-ELEMENTS

NAME	MASS	Z	COEFFICIENTS				
C	32.060	16	0.1402D+01	0.6791D+00	0.5898D+02	0.3528D+01	0.3211D+01
[illegible]	151.000	63	0.1425D+02	0.3630D+00	0.2284D+03	0.7024D+01	0.1816D+01

SPECTRUM NO. 1

290 4401 4690 1104 6800 0 0 0 1
AMOS-FI-SG: BMSD4.SEG57
NAME.....: BOR/SCHE
IMPL.IONS.:
IMPL.FLNCE:
ANAL.IONS.: 4HE
ANAL.DOSE.: 1.25E-7 C
THETA.....: 170 DEG
TARGETPOS.: 29 MM
NOTE1.....: 500 CH./10 V
EXPERIMENT: EU-S/SI ANALYSE
DATE/TIME.: 27: 7:82 / 16:28:21
IMPL.ENERG:
ANALYSIS..: RBS
ALPHA.....: 60DEG
ANAL.ENERG: 2 MEV
MATERIAL..: 1110 A EUS/SI
LOGBOOK...: BMS II/23
NOTE2.....: HV 256X

3859.	3673.	1130.	1700.	3891.	6020.	6800.	6354.	5533.	4955.
4281.	3937.	3685.	3311.	3077.	2865.	2685.	2597.	2273.	2203.
2151.	2070.	2072.	1881.	1927.	1863.	1767.	1755.	1679.	1584.
1615.	1594.	1525.	1475.	1499.	1464.	1430.	1345.	1354.	1354.
1343.	1344.	1280.	1293.	1310.	1224.	1235.	1270.	1191.	1261.
1203.	1171.	1171.	1177.	1142.	1205.	1146.	1156.	1142.	1146.
1118.	1131.	1095.	1043.	1068.	1068.	1084.	1037.	1077.	1084.
1012.	1060.	1025.	1083.	1044.	1011.	992.	1069.	1029.	976.
1022.	959.	1005.	1016.	981.	986.	932.	945.	940.	970.
979.	939.	910.	970.	955.	959.	916.	905.	860.	939.
900.	897.	894.	849.	921.	812.	907.	949.	904.	831.
947.	848.	920.	923.	926.	894.	827.	759.	652.	634.
470.	400.	340.	228.	125.	100.	64.	81.	106.	112.
128.	173.	202.	231.	295.	297.	331.	338.	330.	303.
356.	355.	321.	336.	345.	330.	346.	347.	314.	289.
182.	134.	59.	28.	46.	34.	24.	21.	22.	21.
15.	21.	15.	18.	13.	24.	15.	22.	13.	19.
14.	17.	19.	17.	23.	20.	21.	17.	13.	15.
16.	21.	21.	17.	19.	26.	19.	18.	19.	29.
28.	30.	35.	41.	35.	44.	42.	76.	121.	188.
389.	550.	842.	1219.	1610.	2216.	2749.	3398.	3832.	4348.
4495.	4676.	4598.	4699.	4740.	4505.	4707.	4668.	4606.	4586.
4596.	4605.	4577.	4636.	4299.	3715.	2698.	1364.	379.	77.
8.	8.	4.	7.	6.	0.	2.	5.	2.	3.
4.	1.	5.	3.	1.	5.	2.	2.	1.	1.
2.	0.	1.	0.	2.	3.	0.	1.	3.	3.
0.	1.	3.	1.	3.	2.	4.	2.	0.	1.
1.	2.	0.	1.	1.	2.	2.	1.	0.	1.
2.	2.	0.	2.	1.	1.	1.	0.	0.	

DEPTH	STOCHIOMETRIC COEFFICIENTS,UNCERTAINTIES								CHANNELS						Q
ATOMS/CM2	S	EU							S	EU					
0.0	.538,.04	.462,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	151.	227.	0.	0.	0.	0.	0.189D+
0.250D+17	.546,.03	.454,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	150.	226.	0.	0.	0.	0.	0.285D+
0.501D+17	.525,.03	.475,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	149.	225.	0.	0.	0.	0.	0.335D+
0.747D+17	.523,.03	.477,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	148.	224.	0.	0.	0.	0.	0.367D+
0.993D+17	.525,.03	.475,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	147.	223.	0.	0.	0.	0.	0.373D+
0.124D+18	.518,.03	.482,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	146.	222.	0.	0.	0.	0.	0.368D+
0.148D+18	.499,.03	.501,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	146.	221.	0.	0.	0.	0.	0.364D+
0.172D+18	.502,.03	.498,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	145.	220.	0.	0.	0.	0.	0.361D+
0.196D+18	.513,.03	.487,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	144.	219.	0.	0.	0.	0.	0.364D+
0.221D+18	.509,.03	.491,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	143.	218.	0.	0.	0.	0.	0.365D+
0.245D+18	.526,.03	.474,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	142.	217.	0.	0.	0.	0.	0.376D+
0.269D+18	.529,.03	.471,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	141.	216.	0.	0.	0.	0.	0.367D+
0.293D+18	.487,.03	.513,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	140.	215.	0.	0.	0.	0.	0.354D+
0.317D+18	.504,.03	.496,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	139.	214.	0.	0.	0.	0.	0.364D+
0.341D+18	.515,.03	.485,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	138.	213.	0.	0.	0.	0.	0.362D+
0.365D+18	.511,.03	.489,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	137.	212.	0.	0.	0.	0.	0.361D+
0.389D+18	.497,.03	.503,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	136.	211.	0.	0.	0.	0.	0.346D+
0.412D+18	.496,.03	.504,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	135.	210.	0.	0.	0.	0.	0.333D+
0.436D+18	.489,.03	.511,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	134.	209.	0.	0.	0.	0.	0.299D+
0.459D+18	.474,.03	.526,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	134.	208.	0.	0.	0.	0.	0.259D+
0.482D+18	.487,.04	.513,.01	.0	,.0	.0	,.0	.0	,.0	.0	,.0	133.	207.	0.	0.	0.	0.	0.219D+

Ø.5Ø6D+18	.497,.Ø4	.5Ø3,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	132.	2Ø6.	Ø.	Ø.	Ø.	Ø.	Ø.179D+11
Ø.529D+18	.5Ø2,.Ø4	.498,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	131.	2Ø5.	Ø.	Ø.	Ø.	Ø.	Ø.137D+11
Ø.553D+18	.547,.Ø5	.453,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	13Ø.	2Ø4.	Ø.	Ø.	Ø.	Ø.	Ø.1ØØD+11
Ø.577D+18	.617,.Ø6	.383,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	129.	2Ø3.	Ø.	Ø.	Ø.	Ø.	Ø.86ØD+1Ø
Ø.6Ø2D+18	.655,.Ø7	.345,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	128.	2Ø2.	Ø.	Ø.	Ø.	Ø.	Ø.616D+1Ø
Ø.628D+18	.718,.Ø9	.282,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	127.	2Ø1.	Ø.	Ø.	Ø.	Ø.	Ø.429D+1Ø
Ø.656D+18	.857,.Ø9	.143,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	126.	2ØØ.	Ø.	Ø.	Ø.	Ø.	Ø.438D+1Ø
Ø.687D+18	.925,.Ø9	.Ø75,.Ø1	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	125.	199.	Ø.	Ø.	Ø.	Ø.	Ø.487D+1Ø

TH CONTENTS (ATOMS/CM**2) INTEGRATED FROM SURFACE

EC./CM2	FROM ENERGYLOSS S	EU					I	FROM SCATTERING(DIVIDE BY DOSIS*SOLID-ANGLE) S	EU
	.Ø	.Ø	.Ø	.Ø	.Ø	.Ø		.2Ø5D+27	.131D+27
ØD+17	.135D+17	.115D+17	.Ø	.Ø	.Ø	.Ø		.484D+27	.391D+27
1D+17	.271D+17	.229D+17	.Ø	.Ø	.Ø	.Ø		.925D+27	.746D+27
7D+17	.4Ø1D+17	.347D+17	.Ø	.Ø	.Ø	.Ø		.14ØD+28	.116D+28
3D+17	.529D+17	.464D+17	.Ø	.Ø	.Ø	.Ø		.193D+28	.16ØD+28
4D+18	.658D+17	.581D+17	.Ø	.Ø	.Ø	.Ø		.245D+28	.2Ø3D+28
8D+18	.785D+17	.698D+17	.Ø	.Ø	.Ø	.Ø		.295D+28	.247D+28
2D+18	.9Ø5D+17	.819D+17	.Ø	.Ø	.Ø	.Ø		.34ØD+28	.291D+28
6D+18	.1Ø3D+18	.939D+17	.Ø	.Ø	.Ø	.Ø		.39ØD+28	.334D+28
1D+18	.115D+18	.1Ø6D+18	.Ø	.Ø	.Ø	.Ø		.438D+28	.377D+28
5D+18	.127D+18	.117D+18	.Ø	.Ø	.Ø	.Ø		.491D+28	.42ØD+28
9D+18	.14ØD+18	.129D+18	.Ø	.Ø	.Ø	.Ø		.543D+28	.464D+28
3D+18	.153D+18	.14ØD+18	.Ø	.Ø	.Ø	.Ø		.587D+28	.5Ø5D+28
7D+18	.164D+18	.153D+18	.Ø	.Ø	.Ø	.Ø		.636D+28	.549D+28
1D+18	.177D+18	.164D+18	.Ø	.Ø	.Ø	.Ø		.634D+28	.592D+28
5D+18	.189D+18	.176D+18	.Ø	.Ø	.Ø	.Ø		.684D+28	.633D+28
9D+18	.2Ø1D+18	.188D+18	.Ø	.Ø	.Ø	.Ø		.731D+28	.676D+28
2D+18	.213D+18	.2ØØD+18	.Ø	.Ø	.Ø	.Ø		.774D+28	.716D+28
6D+18	.224D+18	.211D+18	.Ø	.Ø	.Ø	.Ø		.816D+28	.755D+28
9D+18	.236D+18	.223D+18	.Ø	.Ø	.Ø	.Ø		.849D+28	.789D+28
2D+18	.247D+18	.236D+18	.Ø	.Ø	.Ø	.Ø		.877D+28	.819D+28
6D+18	.258D+18	.248D+18	.Ø	.Ø	.Ø	.Ø		.9Ø1D+28	.843D+28
9D+18	.27ØD+18	.259D+18	.Ø	.Ø	.Ø	.Ø		.918D+28	.862D+28
3D+18	.282D+18	.271D+18	.Ø	.Ø	.Ø	.Ø		.932D+28	.875D+28
7D+18	.295D+18	.282D+18	.Ø	.Ø	.Ø	.Ø		.946D+28	.885D+28
2D+18	.311D+18	.292D+18	.Ø	.Ø	.Ø	.Ø		.956D+28	.891D+28
8D+18	.328D+18	.3Ø1D+18	.Ø	.Ø	.Ø	.Ø		.954D+28	.894D+28
6D+18	.347D+18	.3Ø9D+18	.Ø	.Ø	.Ø	.Ø		.962D+28	.895D+28
7D+18	.374D+18	.313D+18	.Ø	.Ø	.Ø	.Ø		.974D+28	.895D+28
ØD+18	.4Ø5D+18	.315D+18	.Ø	.Ø	.Ø	.Ø		.991D+28	.894D+28

We see that taking the 'surface channels' to be no. $\sim$ 151 for S and $\sim$ 227 for Eu we find a surface stoichiometry of $S_{0.538}\ Eu_{0.462}$ within the estimated uncertainties: Because of counting statistics /1/ the stoichiometry may actually be anywhere 'between' $S_{0.578}\ Eu_{0.452}$ and $S_{0.498}\ Eu_{0.472}$. Of course the last digit in each coefficient is meaningless in this case. We note that the two possible 'extreme stoichiometries' above are not normalized (see Section 2.2).

Assuming the stoichiometry to remain constant within the first depthstep, we then find the stoichiometry $S_{0.546}\ Eu_{0.454}$ at depth $2.5 \cdot 10^{16}$ atoms/cm^2 by evaluating channels no. $\sim$ 150 for S and $\sim$ 226 for Eu.

The target composition was evaluated up to a depth of $6.87 \cdot 10^{17}$ atoms/cm^2, corresponding to channels no. $\sim$ 125 for S and $\sim$ 199 for Eu, but a comparison with the spectrum shows this to be too far: Since the substrate (Si) was ignored, it is unreasonable to evaluate the spectrum up to depths where both the S- and the Eu-signals have essentially disappeared.

However, for the purpose of determining the filmthickness we need the integrated peaks from both elements, so here all the evaluated channels count: From the tabulation of the 'integrated contents' vs. depth we now obtain the values (eq. 3.3) $d_S \cdot N_{prim}\Delta\Omega = 0.991 \cdot 10^{28}$ and $d_{Eu} \cdot N_{prim}\Delta\Omega = 0.894 \cdot 10^{28}$. The product $N_{prim}\Delta\Omega$ was determined roughly as $4 \cdot 10^{10}$, but may be estimated better from the heights of the backscattering peaks. We see that the eigenvalue Q varies significantly within the first channels/depth steps, reflecting the effect of experimental resolution. However, for the channels corresponding to the peak-plateaus the eigenvalue remains almost constant around $3.65 \cdot 10^{10}$. Using this value for $N_{prim}\Delta\Omega$ we thus have $\sim 2.72 \cdot 10^{17}$ S/cm^2 and $2.45 \cdot 10^{17}$ Eu/cm^2 in the target, i.e. a total of $\sim 5.17 \cdot 10^{17}$ atoms/cm^2.

Going back to the targetcomposition vs. depth we then ignore depths larger than $5.1 \cdot 10^{17}$ atoms/cm^2, and end up with the result shown in Fig. 7.

The program also provides a list of the results on an output-segment specified in the job control cards (Sect. 6.2). This segment (discussed and used further in the next example) may be used as input for our plotting programs.

2. The next example demonstrates the use of a particular facility:
The inclusion of results from previous runs.

a) First a qualitative investigation done without the program. The target was supposed to consist of 3 layers: 1080 Å of EuS on top of a 680 Å SrS-film, all on a Si-substrate. In Rutherford backscattering analysis reasonable depth resolution could be obtained using 2 MeV $^4He^+$-ions and tilting the target. Unfortunately, signals from Si near the surface would be superposed on the S-signal from larger depths.

There is not supposed to be any Si near the surface, but in order to check this, a spectrum was first measured with 2.5 MeV $^4He^+$-ions at an incident angle $\alpha = 15^o$ (Fig. 8). In this spectrum the depth resolution was poor, but it was clearly seen that there is no Si near the surface. Instead a small peak was found, indicating 5-10 % Sr at the surface.

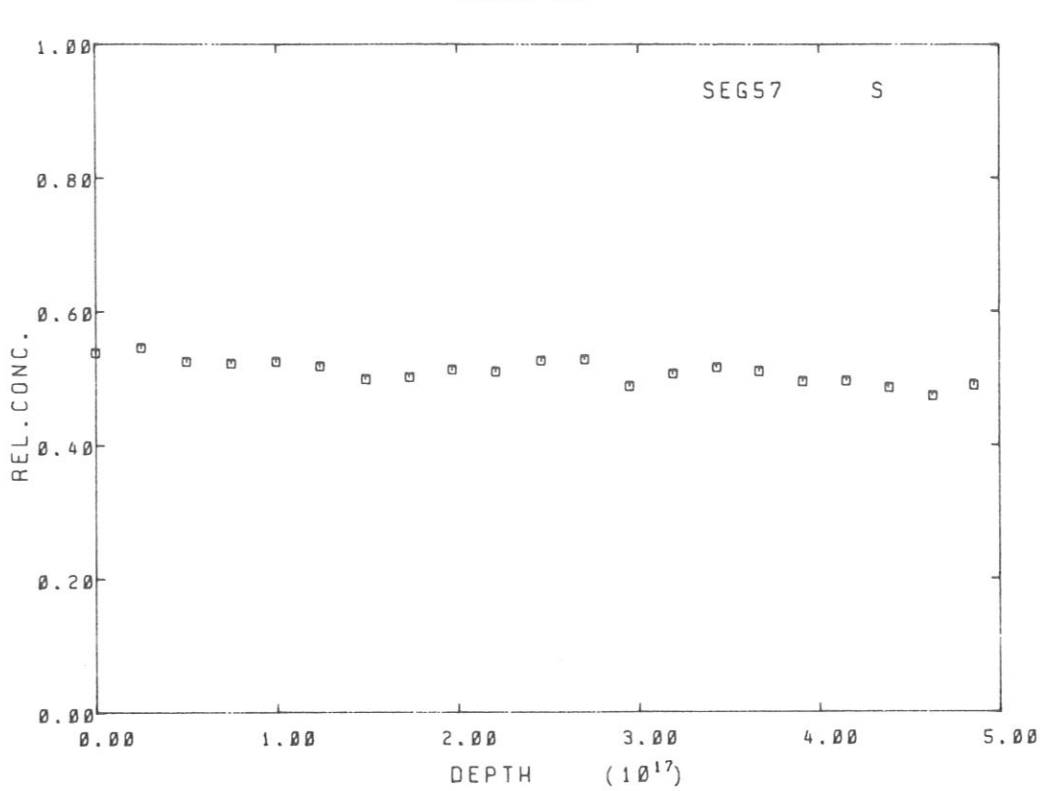


Fig. 7a: Plot of SQUEAKIE - output resulting from evaluation of spectrum in Fig.6. Original SQUEAKIE-version. Relative concentration vs. depth of S.

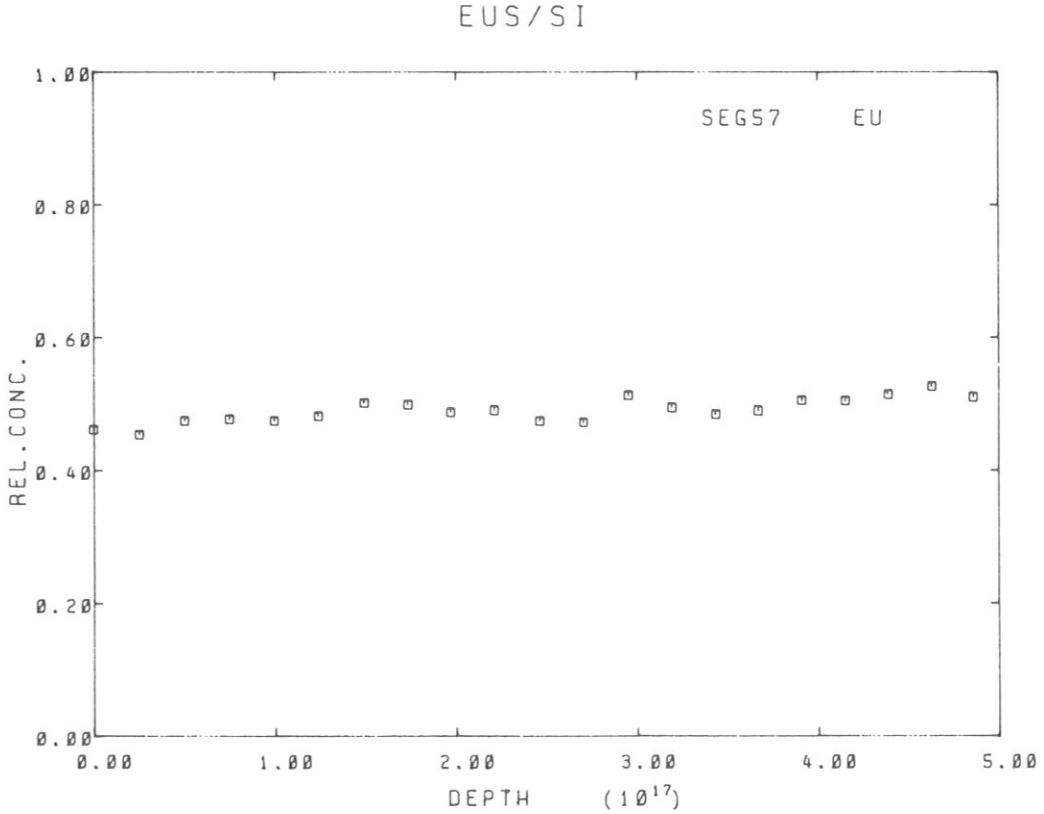


Fig. 7b: Relative concentration vs. depth of Eu

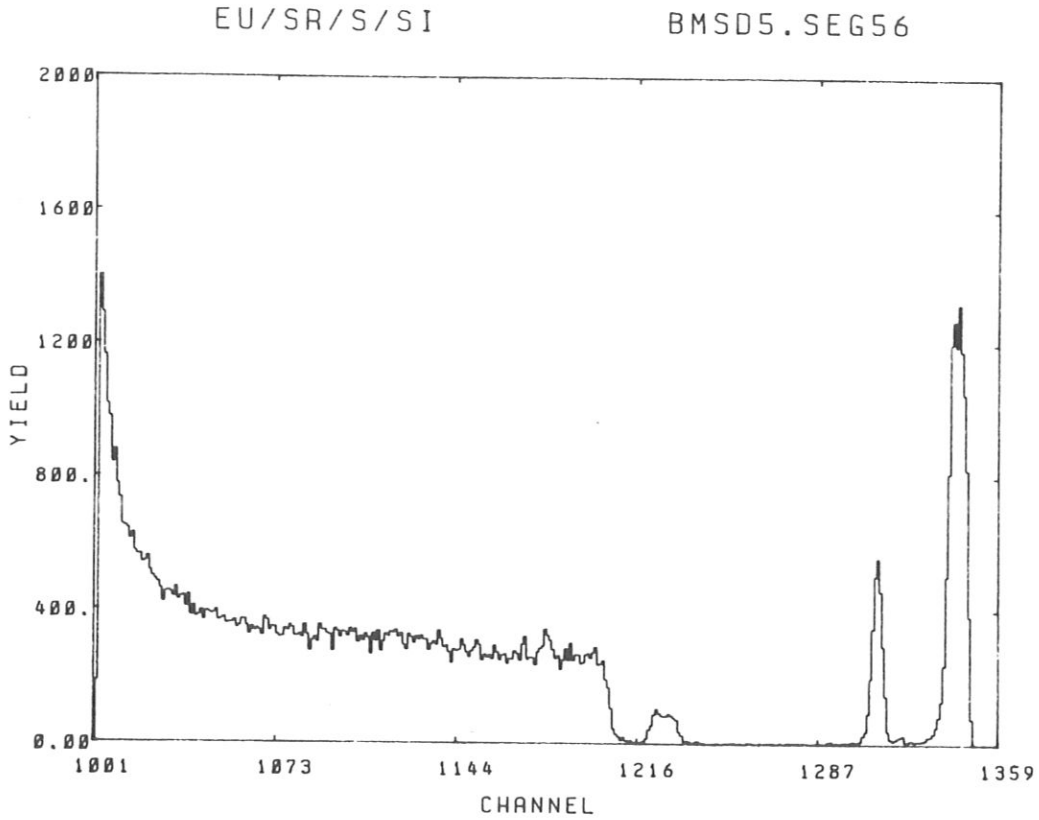


Fig. 8: RBS-spectrum for 2.5 MeV ^{4}He-ions scattered from 1080 Å EuS / 680 Å SrS/Si.

b) An experimental spectrum was now obtained using 2 MeV $^{4}He^{+}$-ions and a (laboratory) scattering angle θ of 165^{o} (Fig. 9). The target was tilted an angle $\alpha = 15^{o}$ perpendicular to the scattering plane, giving the detectorangle $\beta \sim 21.1^{o}$.

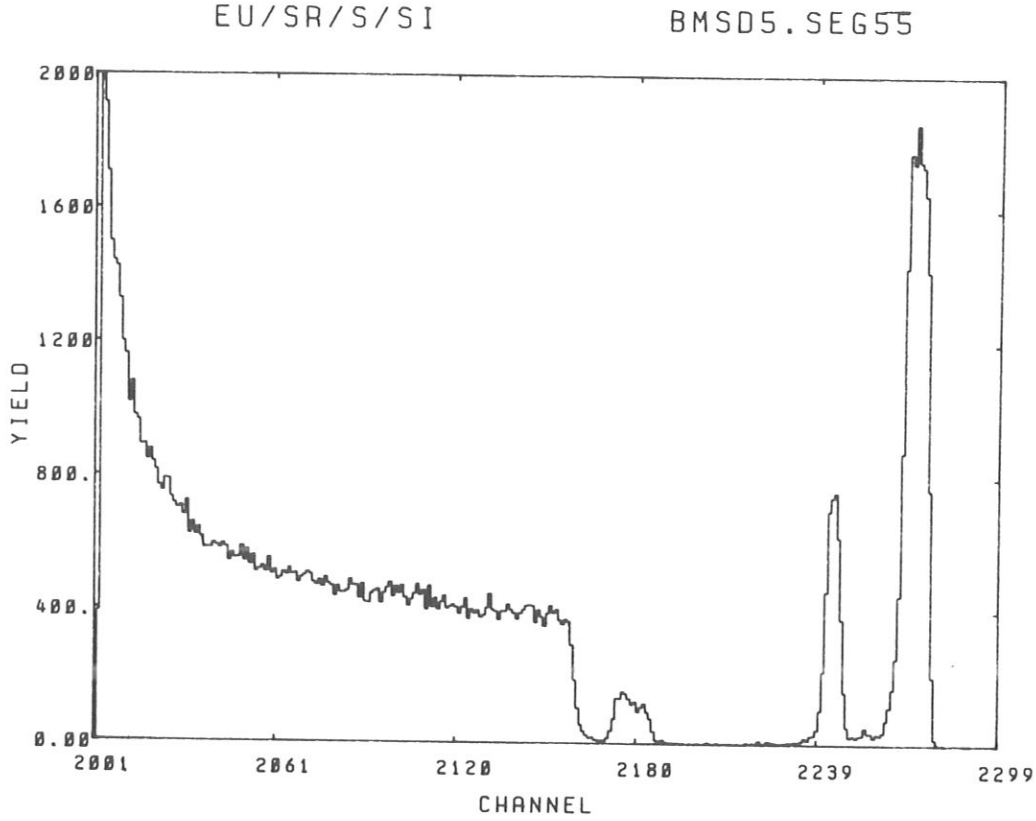


Fig. 9: RBS-spectrum for 2 MeV ^{4}He-ions scattered from 1080 Å EuS / 680 Å SrS/Si
$\theta = 165^{\circ}$, $\alpha = 15^{\circ}$, $\beta = 21.1^{\circ}$

The energy calibration used was

$$E_{det} = ch \times 6.3909 + 41.172$$

where 'ch' is the channelnumber, and E_{det} is the corresponding energy in keV.

As noted above, signals from Si near the surface would be superposed on the S-signal from larger depths. We know that there is no Si-signal superposed on the S-signal, but the program is not capable of distinguishing this. In the Aarhus-version this is handled by defining appropriate markers

(see Sect. 5.9), here we first analyze the near-surface layer, looking only for the other three elements:

In the listed input-example (below) the calculations are to be terminated at the depth x, where the inward beam energy becomes less than 1000.0 keV, or from which one of the experimental signals falls in a channel below 181 .In the present case this happens when the S-signal corresponds to a channel slightly below 181 (see output).

In the present calculations, the integrated contents are not of interest.

We expect to find three different target elements at the present depths: S, Eu, and Sr.
Only one experimental spectrum, containing 299 channels, is to be evaluated in this run.
For each of the three possible targetelements the appropriate ^{4}He-stopping power coefficients are taken from Ref. 11.

Input:

```
165.Ø      15.Ø       21.1
2ØØØ.      6.39Ø9     +41.172
1ØØØ.Ø     181    Ø 2 Ø
 3
 1    299
4.ØØ16          2    1.Ø
32.Ø6          16    S
1.4Ø2      E+Ø 6.791      E-1 5.898      E+1 3.528      E+Ø 3.211      E+Ø
152.Ø          63    EU
1.422      E+1 3.63       E-1 2.284      E+2 7.Ø24      E+Ø 1.Ø16      E+Ø
87.63          38    SR
7.126      E+Ø 4.ØØ4      E-1 1.193      E+2 5.784      E+Ø 2.454      E+Ø


   299   2ØØ1    2299      17   21Ø2      Ø      Ø      Ø      1
AMOS-FI-SG: BMSD5.SEG55          EXPERIMENT: EU/SR/S/SI
NAME......: BOE/SCHE             DATE/TIME.: 27: 8:82 / 11: 9:19
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 15 DEG
ANAL.DOSE.: 2ØE-6 C              ANAL.ENERG: 2 MEV
THETA.....: 165 DEG              MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X       NOTE2.....: 1ØØØ CH/1Ø V
     Ø    392   21Ø2   1912   17Ø7   1497   1439   1423   1326   1197
  1161   1Ø16   1Ø79    977    964    89Ø    893    846    878    839
   814    768    753    79Ø    788    733    715    7Ø2    7Ø8    681
   725    624    66Ø    622    644    615    582    584    583    598
   59Ø    582    595    586    544    567    553    554    58Ø    544
   579    533    561    512    52Ø    529    512    554    5Ø6    517
   488    495    513    5Ø3    525    5Ø5    5Ø8    48Ø    497    5Ø4
   513    5Ø6    48Ø    474    488    469    496    477    47Ø    44Ø
   47Ø    452    452    459    492    472    472    434    478    421
   42Ø    45Ø    456    461    42Ø    451    467    4Ø3    439    471
   449    474    436    412    432    45Ø    477    444    458    4ØØ
   473    4Ø7    436    4Ø1    426    443    4Ø4    412    417    4Ø8
   389    4Ø9    436    373    4Ø2    391    399    379    386    4Ø8
   449    4ØØ    396    372    397    397    419    4ØØ    39Ø    373
   393    4Ø3    415    416    413    363    4ØØ    38Ø    352    393
   414    392    4Ø2    369    358    373    366    295    19Ø    1Ø5
    57     38     25     16     2Ø     11      9      9      9     18
    41     77    139    136    158    151    134    118    126     97
   11Ø    12Ø     95     76     38     11      9     13      6      4
     5      2      5      1      3      Ø      3      Ø      3      3
     Ø      3      6      3      1      4      1      2      3      2
     3      1      2      1      1      6      3      6      3     13
     5      4     12      8      6      5      2      4      6      8
     7      9      8     13     21     15     29     31     47    1Ø6
   222    462    7Ø4    744    757    621    377    158     53     23
    28     22     28     31     53     35     35     23     34     3Ø
    39     76    114    17Ø    261    45Ø    879   1432   1775   1744
  1861   1749   1733   1647   1418    764    2Ø4     19      2      Ø
     1      Ø      Ø      Ø      Ø      Ø      Ø      1      1      Ø
     Ø      Ø      Ø      Ø      Ø      Ø      Ø      Ø      Ø
```

On the output we find, after a list of the input, a table of the stoichiometric coefficients vs. depth (see also previous example).

We see that taking the surface channels to be no. ∿ 185 for S, no. ∿ 276 for Eu and no. ∿ 255 for Sr the surface stoichiometry is evaluated as $S_{0.413}\ Eu_{0.51}\ Sr_{0.076}$ within the estimated uncertainties. Assuming the stoichiometry to remain constant within the first depthstep, we then find the stoichiometry $S_{0.434}\ Eu_{0.535}\ Sr_{0.031}$ at depth $3.77 \cdot 10^{16}$ atoms/cm^2 by evaluating channels no . ∿ 184 for S, no. ∿ 275 for Eu and no. ∿ 254 for Sr.

The targetcomposition was first only evaluated up to a depth of $1.14 \cdot 10^{17}$ atoms/cm^2.

We note that the eigenvalue Q varies significantly within the first channels/depthsteps, reflecting the effect of experimental resolution. However, the presence of ∿ 8 % Sr on the surface is at least approximately correct, indicating a partial 'cancellation of errors' /1/.

```
 SCATTERING ANGLE =   165.Ø , INC.ANGLE =    15.Ø AND EXIT-ANGLE =    21.1 DEGREES
 INCIDENT ENERGY =   2ØØØ. KEV,    6.391 KEV/CHANNEL,  AND ENERGY =   41.172 IN CHANNEL Ø
 STOP EVALUATION WHEN EBEAM<  1ØØØ. KEV, OR WHEN CHANNELS BELOW CH. 181 ARE REQUESTED
  1 SPECTRA ARE EVALUATED WITH THIS INPUT
 PROJECTILE HAS MASS =      4.ØØ2, AND Z =  2
  ENERGY-SCALING FACTOR      1.ØØØ

             TARGET-ELEMENTS
             ---------------
NAME    MASS          Z                          COEFFICIENTS

 S       32.Ø6Ø       16     Ø.1482D+Ø1    Ø.6791D+ØØ    Ø.5898D+Ø2    Ø.3528D+Ø1    Ø.3211D+Ø1
EU      152.ØØØ       63     Ø.1422D+Ø2    Ø.363ØD+ØØ    Ø.2284D+Ø3    Ø.7Ø24D+Ø1    Ø.1Ø16D+Ø1
SR       87.63Ø       38     Ø.7126D+Ø1    Ø.4804D+ØØ    Ø.1193D+Ø3    Ø.5784D+Ø1    Ø.2454D+Ø1
```

```
SPECTRUM NO.  1

   299    2001    2299      17    2102       0       0       0       1
AMOS-FI-SG: BMSD5.SEG55              EXPERIMENT: EU/SR/S/SI
NAME.....: BOE/SCHE                  DATE/TIME.: 27: 8:82 / 11: 9:19
IMPL.IONS.:                          IMPL.ENERG:
IMPL.FLNCE:                          ANALYSIS..: RBS
ANAL.IONS.: 4HE                      ALPHA.....: 15 DEG
ANAL.DOSE.: 20E-6 C                  ANAL.ENERG: 2 MEV
THETA.....: 165 DEG                  MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                    LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X            NOTE2.....: 1000 CH/10 V
     0.      392.    2102.    1912.    1707.    1497.    1439.    1423.    1326.    1197.
  1151.    1016.    1079.     977.     964.     890.     893.     846.     878.     839.
   814.     768.     753.     790.     788.     733.     715.     702.     708.     681.
   725.     624.     660.     622.     644.     615.     582.     584.     583.     598.
   590.     582.     595.     586.     544.     567.     553.     554.     588.     544.
   579.     533.     561.     512.     520.     529.     512.     554.     506.     517.
   488.     495.     513.     503.     525.     505.     508.     480.     497.     504.
   513.     506.     480.     474.     488.     469.     496.     477.     470.     440.
   470.     452.     452.     459.     492.     472.     472.     434.     478.     421.
   420.     450.     456.     461.     420.     451.     467.     483.     439.     471.
   449.     474.     436.     412.     432.     450.     477.     444.     458.     400.
   473.     407.     436.     401.     426.     443.     404.     412.     417.     408.
   389.     409.     436.     373.     402.     391.     399.     379.     386.     408.
   449.     400.     396.     372.     397.     397.     419.     400.     390.     373.
   393.     403.     415.     416.     413.     363.     400.     380.     352.     393.
   414.     392.     402.     369.     358.     373.     366.     295.     190.     105.
    57.      38.      25.      16.      20.      11.       9.       9.       9.      18.
    41.      77.     139.     136.     158.     151.     134.     118.     126.      97.
   110.     120.      95.      76.      38.      11.       9.      13.       6.       4.
     5.       2.       5.       1.       3.       0.       3.       0.       3.       3.
     0.       3.       6.       3.       1.       4.       1.       2.       3.       2.
     3.       1.       2.       1.       1.       6.       3.       6.       3.      13.
     5.       4.      12.       8.       6.       5.       2.       4.       6.       8.
     7.       9.       8.      13.      21.      15.      29.      31.      47.     106.
   222.     462.     704.     744.     757.     621.     377.     158.      53.      23.
    28.      22.      28.      31.      53.      35.      35.      23.      34.      30.
    39.      76.     114.     170.     261.     450.     879.    1432.    1775.    1744.
  1861.    1749.    1733.    1647.    1418.     764.     204.      19.       2.       0.
     1.       0.       0.       0.       0.       0.       0.       1.       1.       0.
     0.       0.       0.       0.       0.       0.       0.       0.       0.

  DEPTH          STOCHIOMETRIC COEFFICIENTS,UNCERTAINTIES                                  CHANNELS                          Q
  ATOMS/CM2      S          EU          SR                                                 S     EU    SR

  0.0        .413,.006  .510,.002  .076,.001  .0  ,.0  .0  ,.0  .0  ,.0   185.  276.  255.   0.    0.    0.   0.910D+18
  0.377D+17  .434,.005  .535,.001  .031,.001  .0  ,.0  .0  ,.0  .0  ,.0   184.  275.  254.   0.    0.    0.   0.136D+11
  0.756D+17  .459,.005  .517,.001  .023,.000  .0  ,.0  .0  ,.0  .0  ,.0   183.  274.  253.   0.    0.    0.   0.156D+11
  0.114D+18  .491,.005  .492,.001  .017,.000  .0  ,.0  .0  ,.0  .0  ,.0   182.  273.  252.   0.    0.    0.   0.166D+11
```

Besides from the printed output, the program also provides a list of the results on an outputsegment which was specified in the job control cards (For example 1 in Sect. 6.2 the results are tabulated on the segment PRB: B.EUS55). A listing of the outputsegment is shown below. The format has been chosen so that this segment may be used as input in the next run, as well as for our plotting programs:

```
   299    2001    2299      17    2102       0       0       0       1
AMOS-FI-SG: BMSD5.SEG55              EXPERIMENT: EU/SR/S/SI
NAME.....: BOE/SCHE                  DATE/TIME.: 27: 8:82 / 11: 9:19
IMPL.IONS.:                          IMPL.ENERG:
IMPL.FLNCE:                          ANALYSIS..: RBS
ANAL.IONS.: 4HE                      ALPHA.....: 15 DEG
ANAL.DOSE.: 20E-6 C                  ANAL.ENERG: 2 MEV
THETA.....: 165 DEG                  MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                    LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X            NOTE2.....: 1000 CH/10 V
                    S          EU          SR
      0.0        0.413      0.510      0.076      0.0        0.0        0.0
      0.377D+17  0.434      0.535      0.031      0.0        0.0        0.0
      0.756D+17  0.459      0.517      0.023      0.0        0.0        0.0
      0.114D+18  0.491      0.492      0.017      0.0        0.0        0.0
```

c. Still another experimental spectrum was obtained using 2 MeV $^4He^+$-ions and $\theta = 165^o$. This time the depthresolution was improved by tilting the target an angle $\alpha = 60^o$ perpendicular to the scattering plane (Fig. 10). Thus the detectorangle $\beta \simeq 61.1^o$.

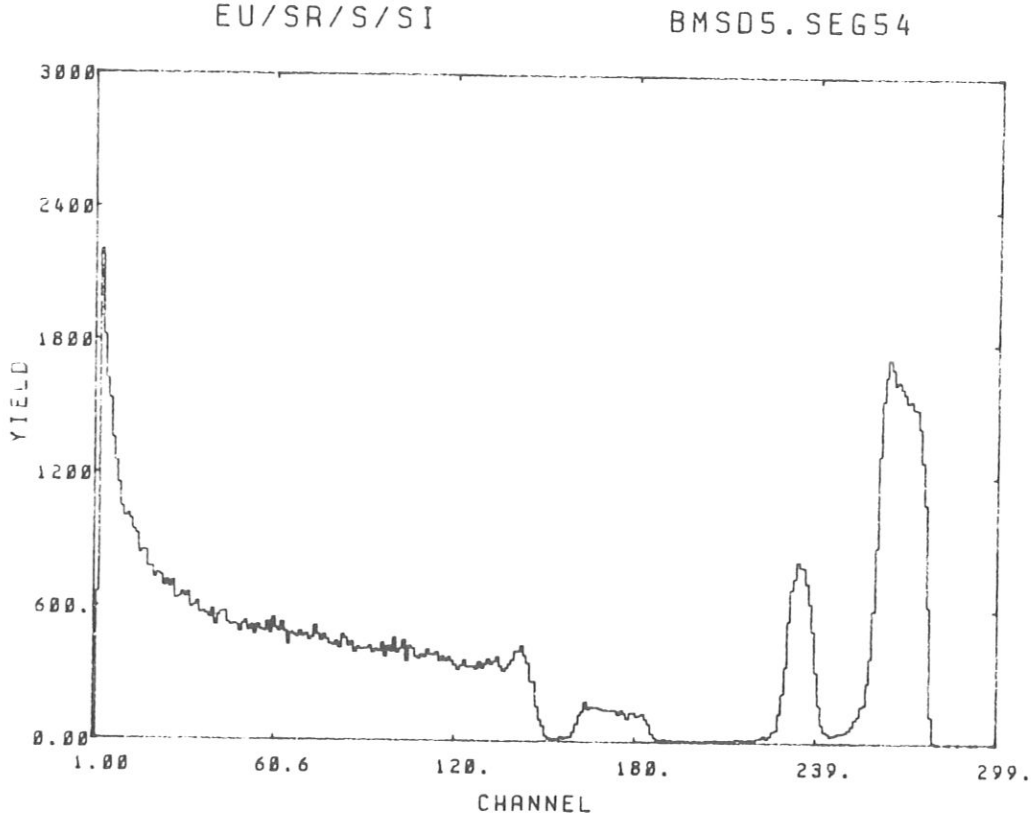


Fig. 10: RBS-spectrum for 2 MeV ^4He-ions scattered from 1080 Å EuS/ 680 Å SrS/Si
$\theta = 165^o$, $\alpha = 60^o$, $\beta = 61.1^o$.

Unfortunately the tilting made the small Sr-peak from the surface (see Figs. 8 and 9) disappear in the 'tail' of the Eu-peak, so we may now not correctly evaluate the surface layer from this spectrum. Instead we read in the results from the previous run (residing on segment PRB: B.EUS55,

(see above), and only evaluate the present spectrum for depths larger than $1.14 \cdot 10^{17}$ atoms/cm^2. We thus remember to link the segment PRB: B.EUS55 to the data in the inputstream (see example 2, sect.6.2), and define a new outputsegment PRB: B.EU355.

We are still considering quite shallow depths from which a Si-signal would be superposed on the S-signal (see above). We therefore still only look for the three targetelements S, Eu and Sr up to such depths, from which the S-signal falls in channels below 166.

The necessary input was:

```
165.Ø      6Ø.Ø       61.1
2ØØØ.      6.39Ø9     +4i.172
1ØØØ.Ø     166    Ø 2 1
 3
 1    299
4.ØØ16          2    1.Ø
32.Ø6          16    S
1.4Ø2      E+Ø 6.791      E-1 5.898      E+1 3.528      E+Ø 3.211      E+Ø
152.Ø          63   EU
1.4Ø2      E+1 3.63       E-1 2.284      E+2 7.Ø24      E+Ø 1.Ø16      E+Ø
87.63          38   Sr
7.126      E+Ø 4.8Ø4      E-1 1.193      E+2 5.784      E+Ø 2.454      E+Ø
```

```
   299       1     299       Ø    22Ø6       Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG54              EXPERIMENT: EU/SR/S/SI
NAME......: BOE/SCHE                 DATE/TIME.: 27: 8:82 / 1Ø:45:55
IMPL.IONS.:                          IMPL.ENERG:
IMPL.FLNCE:                          ANALYSIS..: RBS
ANAL.IONS.: 4HE                      ALPHA.....: 6Ø
ANAL.DOSE.: 2ØE-6 C                  ANAL.ENERG: 2 MEV
THETA.....: 165 DEG                  MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                    LOGBOOK...: RBS V1/175
NOTE1.....: H.V.GAIN=256X            NOTE2.....: 1ØØØ CH/1Ø V
      Ø      663     22Ø6     182Ø     162Ø     1533     1356     1251     1151     1Ø45
   1ØØ4     1Ø14      99Ø      941      921      836      851      851      775      775
    73Ø      75Ø      739      692      719      687      717      636      643      663
    643      665      596      6Ø7      624      573      579      568      552      592
    518      565      577      581      527      518      522      516      488      526
    538      494      519      476      52Ø      497      493      533      481      554
    5Ø6      492      533      49Ø      433      486      475      465      492      468
    478      453      465      517      476      45Ø      478      454      435      429
    448      418      478      46Ø      426      446      399      424      413      415
    415      43Ø      397      414      4Ø2      443      379      427      4Ø4      466
    399      416      453      359      429      415      38Ø      372      389      379
    414      39Ø      387      4ØØ      362      381      36Ø      38Ø      362      342
    323      343      367      336      334      339      326      359      329      351
    372      349      361      382      338      316      333      351      37Ø      4Ø9
    4Ø8      434      388      354      27Ø      271      159      1ØØ       73       28
     1Ø       13       14       14       25       16       23       26       47       85
    123      14Ø      1ØØ      147      157      155      156      151      146      145
    143      144      145      125      146      129      1Ø5      134      134      117
    121      12Ø      1Ø2       82       39       19       11        7       17        Ø
     11        7        7        Ø       1Ø        9        7        3       1Ø        5
      6        5        Ø       1Ø       1Ø       11        7        9        Ø       1Ø
     11        7       17       16       14       12       16       15       12       22
     26       34       23       36       55       62      136      226      348      554
    694      745      819      794      792      721      63Ø      5Ø5      321      173
     85       53       46       32       39       42       47       47       53       65
     83      112      126      168      176      275      388      6Ø2      886     13Ø1
   155Ø     1657     1736     1691     1619     1634     16Ø1     1576     154Ø     1545
   151Ø     15Ø7     1425     1272     1Ø78      617      125        9        2        Ø
      Ø        1        1        Ø        Ø        1        Ø        Ø        Ø        1
      Ø        1        Ø        Ø        Ø        Ø        Ø        Ø        1
```

```
   299   2ØØ1   2299      17   21Ø2       Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG55              EXPERIMENT: EU/SR/S/SI
NAME......: BOE/SCHE                 DATE/TIME.: 27: 8:82 / 11: 9:19
IMPL.IONS.:                          IMPL.ENERG:
IMPL.FLNCE:                          ANALYSIS..: RBS
ANAL.IONS.: 4HE                      ALPHA.....: 15 DEG
ANAL.DOSE.: 2ØE-6 C                  ANAL.ENERG: 2 MEV
THETA.....: 165 DEG                  MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                    LOGBOOK...: PBS V1/175
NOTE1.....: H.V.GAIN=256X            NOTE2.....: 1ØØØ CH/1Ø V
                    S       EU       SR
      Ø.Ø           Ø.413    Ø.51Ø    Ø.Ø76    Ø.Ø      Ø.Ø      Ø.Ø
    Ø.377D+17       Ø.434    Ø.535    Ø.Ø31    Ø.Ø      Ø.Ø      Ø.Ø
    Ø.756D+17       Ø.459    Ø.517    Ø.Ø23    Ø.Ø      Ø.Ø      Ø.Ø
    Ø.114D+18       Ø.491    Ø.492    Ø.Ø17    Ø.Ø      Ø.Ø      Ø.Ø
```

The output is on the same form as before, only the results now extend up to the depth $3.85 \cdot 10^{17}$ atoms/cm^2 (the tabulation on the output-segment PRB: B.EU355 of course also). As expected, the eigenvalue Q now varies much less.

```
SCATTERING ANGLE =   165.Ø , INC.ANGLE =    6Ø.Ø AND EXIT-ANGLE =    61.1 DEGREES

INCIDENT ENERGY =   2ØØØ. KEV,    6.391 KEV/CHANNEL,  AND ENERGY =   41.172 IN CHANNEL Ø

STOP EVALUATION WHEN EBEAM<   1ØØØ. KEV, OR WHEN CHANNELS BELOW CH. 166 ARE REQUESTED

 1 SPECTRA ARE EVALUATED WITH THIS INPUT

PROJECTILE HAS MASS =      4.ØØ2, AND Z =  2
 ENERGY-SCALING FACTOR     1.ØØØ

            TARGET-ELEMENTS
            ---------------

NAME    MASS          Z                                  COEFFICIENTS

 S       32.Ø6Ø       16      Ø.14Ø2D+Ø1      Ø.6791D+ØØ      Ø.5898D+Ø2      Ø.3528D+Ø1      Ø.3211D+Ø1
EU      152.ØØØ       63      Ø.1422D+Ø2      Ø.3638D+ØØ      Ø.2284D+Ø3      Ø.7Ø24D+Ø1      Ø.1Ø16D+Ø1
SR       87.63Ø       38      Ø.7126D+Ø1      Ø.4804D+ØØ      Ø.1193D+Ø3      Ø.5784D+Ø1      Ø.2454D+Ø1

            SPECTRUM NO.  1

  299       1    299      Ø   2286      Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG54                 EXPERIMENT: EU/SR/S/SI
NAME.....: BOE/SCHE                     DATE/TIME.: 27: 8:82 / 1Ø:45:55
IMPL.IONS.:                             IMPL.ENERG:
IMPL.FLNCE:                             ANALYSIS..: RBS
ANAL.IONS.: 4HE                         ALPHA.....: 6Ø
ANAL.DOSE.: 2ØE-6 C                     ANAL.ENERG: 2 MEV
THETA.....: 165 DEG                     MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                       LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X               NOTE2.....: 1ØØØ CH/1Ø V
    Ø.     663.    2286.   1828.    1628.   1533.   1356.   1251.   1151.   1Ø45.
 1ØØ4.    1Ø14.    99Ø.    941.     921.    836.    851.    851.    775.    775.
  73Ø.     75Ø.    739.    692.     719.    687.    717.    636.    643.    663.
  643.     665.    596.    6Ø7.     624.    573.    579.    568.    552.    592.
  518.     565.    577.    581.     527.    518.    522.    516.    488.    526.
  538.     494.    519.    476.     52Ø.    497.    493.    533.    481.    554.
  5Ø6.     492.    533.    49Ø.     433.    486.    475.    465.    492.    468.
  478.     453.    465.    517.     476.    45Ø.    478.    454.    435.    429.
  448.     418.    478.    46Ø.     426.    446.    399.    424.    413.    415.
  415.     43Ø.    397.    414.     4Ø2.    443.    379.    427.    4Ø4.    466.
  399.     416.    453.    359.     429.    415.    38Ø.    372.    389.    379.
  414.     39Ø.    387.    4ØØ.     362.    381.    36Ø.    38Ø.    362.    342.
  323.     343.    367.    336.     334.    339.    326.    359.    329.    351.
  372.     349.    361.    382.     338.    316.    333.    351.    37Ø.    4Ø9.
  4Ø8.     434.    388.    354.     27Ø.    271.    159.    1ØØ.     73.     28.
   18.      13.     14.     14.      25.     16.     23.     26.     47.     85.
  123.     14Ø.    18Ø.    147.     157.    155.    156.    151.    146.    145.
  143.     144.    145.    125.     146.    129.    1Ø5.    134.    134.    117.
  121.     128.    1Ø2.     82.      39.     19.     11.      7.     17.      8.
   11.       7.      7.      8.      1Ø.      9.      7.      3.     1Ø.      5.
    6.       5.      8.     1Ø.      1Ø.     11.      7.      9.      8.     1Ø.
   11.       7.     17.     16.      14.     12.     16.     15.     12.     22.
   26.      34.     23.     36.      55.     62.    136.    226.    348.    554.
  694.     745.    819.    794.     792.    721.    63Ø.    5Ø5.    321.    173.
   85.      53.     46.     32.      39.     42.     47.     47.     53.     65.
   83.     112.    126.    168.     176.    275.    388.    6Ø2.    886.   13Ø1.
 1558.    1657.   1736.   1691.    1619.   1634.   16Ø1.   1576.   154Ø.   1545.
 1518.    1587.   1425.   1272.    1Ø78.    617.    125.      9.      2.      Ø.
    Ø.       1.      1.      Ø.       Ø.      1.      Ø.      Ø.      Ø.      1.
    Ø.       1.      Ø.      Ø.       Ø.      Ø.      Ø.      Ø.      1.

 DEPTH          STOCHIOMETRIC COEFFICIENTS,UNCERTAINTIES                    CHANNELS                    Q
 ATOMS/CM2      S          EU          SR                                   S    EU    SR

 Ø.Ø          .413        .518        .Ø76        .Ø          .Ø          .Ø
 Ø.377D+17    .434        .535        .Ø31        .Ø          .Ø          .Ø
 Ø.756D+17    .459        .517        .Ø23        .Ø          .Ø          .Ø
 Ø.114D+18    .491        .492        .Ø17        .Ø          .Ø          .Ø
 Ø.152D+18    .5ØØ,.Ø5    .462,.Ø1    .Ø37,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   177.  268.  247.   Ø.    Ø.    Ø.   Ø.157D
 Ø.173D+18    .5Ø2,.Ø5    .464,.Ø1    .Ø34,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   176.  267.  246.   Ø.    Ø.    Ø.   Ø.159D
 Ø.193D+18    .538,.Ø5    .434,.Ø1    .Ø29,.ØØ    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   175.  266.  245.   Ø.    Ø.    Ø.   Ø.168D
 Ø.214D+18    .538,.Ø5    .438,.Ø1    .Ø25,.ØØ    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   175.  265.  244.   Ø.    Ø.    Ø.   Ø.167D
 Ø.235D+18    .519,.Ø4    .451,.Ø1    .Ø3Ø,.ØØ    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   174.  264.  243.   Ø.    Ø.    Ø.   Ø.178D
 Ø.256D+18    .534,.Ø4    .431,.Ø1    .Ø35,.ØØ    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   173.  263.  242.   Ø.    Ø.    Ø.   Ø.177D
 Ø.277D+18    .536,.Ø4    .412,.Ø1    .Ø52,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   172.  262.  241.   Ø.    Ø.    Ø.   Ø.174D
 Ø.298D+18    .53Ø,.Ø4    .369,.Ø1    .1Ø2,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   171.  261.  24Ø.   Ø.    Ø.    Ø.   Ø.174D
 Ø.319D+18    .527,.Ø4    .284,.Ø1    .189,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   17Ø.  26Ø.  239.   Ø.    Ø.    Ø.   Ø.174D
 Ø.341D+18    .518,.Ø4    .185,.Ø1    .297,.Ø1    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   169.  259.  238.   Ø.    Ø.    Ø.   Ø.175D
 Ø.363D+18    .513,.Ø4    .117,.Ø1    .37Ø,.Ø2    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   168.  258.  237.   Ø.    Ø.    Ø.   Ø.18ØD
 Ø.385D+18    .5Ø9,.Ø4    .Ø74,.ØØ    .417,.Ø2    .Ø  ,.Ø     .Ø  ,.Ø     .Ø  ,.Ø   167.  257.  236.   Ø.    Ø.    Ø.   Ø.184D
```

d. Finally we have now evaluated the spectrum to such depths, that we may soon expect the presence of Si (see above). We therefore look for all 4 elements (S, Eu, Sr, and Si) at depths larger than $3.85 \cdot 10^{17}$ atoms/cm^2. The targetcomposition for depths up to $3.85 \cdot 10^{17}$ atoms/cm^2 is read in from the segment PRB: B.EU355, see above.

The rest of the input remains the same, except that we now evaluate the spectrum up to such depths, from which the Si-signal falls in channels below 130:

```
165.Ø      6Ø.Ø       61.1
1ØØØ.      6.39Ø9     +41.172
1ØØØ.Ø     13Ø    Ø 2 1
 4
 1     299
4.ØØ16          2    1.Ø
32.Ø6          16    S
1.4Ø2      E+Ø 6.791      E-1 5.898Ø      E+1 3.528      E+Ø 3.211      E+Ø
152.Ø          63   EU
1.422      E+1 3.63       E-1 2.284       E+2 7.Ø24      E+Ø 1.Ø16      E+Ø
87.63          38   SR
7.126      E+Ø 4.8Ø4      E-1 1.193       E+2 5.784      E+Ø 2.454      E+Ø
28.Ø6          14   SI
2.1        E+Ø 6.5        E-1 4.934       E+1 1.788      E+Ø 4.133      E+Ø
```

```
   299      1    299       Ø    22Ø6       Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG54          EXPERIMENT: EU/SR/S/SI
NAME......: BOE/SCHE             DATE/TIME.: 27: 8:82 / 1Ø:45:55
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 6Ø
ANAL.DOSE.: 2ØE-6 C              ANAL.ENERG: 2 MEV
THETA.....: 165 DEG              MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X        NOTE2.....: 1ØØØ CH/1Ø V
     Ø     663    22Ø6    182Ø    162Ø    1533    1356    1251    1151    1Ø45
  1ØØ4    1Ø14     99Ø     941     921     836     851     851     775     775
   73Ø     75Ø     739     692     719     687     717     636     643     663
   643     665     596     6Ø7     624     573     579     568     552     592
   518     565     577     581     527     518     522     516     488     526
   538     494     519     476     52Ø     497     493     533     481     554
   5Ø6     492     533     49Ø     433     486     475     465     492     468
   478     453     465     517     476     45Ø     478     454     435     429
   448     418     478     46Ø     426     446     399     424     413     415
   415     43Ø     397     414     4Ø2     443     379     427     4Ø4     466
   399     416     453     359     429     415     38Ø     372     389     379
   414     39Ø     387     4ØØ     362     381     36Ø     38Ø     362     342
   323     343     367     336     334     339     326     359     329     351
   372     349     361     382     338     316     333     351     37Ø     4Ø9
   4Ø8     434     388     354     27Ø     271     159     1ØØ      73      28
    18      13      14      14      25      16      23      26      47      85
   123     14Ø     1ØØ     147     157     155     156     151     146     145
   143     144     145     125     146     129     1Ø5     134     134     117
   121     12Ø     1Ø2      82      39      19      11       7      17       Ø
    11       7       7       8      1Ø       9       7       3      1Ø       5
     6       5       8      1Ø      1Ø      11       7       9       Ø      1Ø
    11       7      17      16      14      12      16      15      12      22
    26      34      23      36      55      62     136     226     348     554
   694     745     819     794     792     721     63Ø     5Ø5     321     173
    85      53      46      32      39      42      47      47      53      65
    83     112     126     168     176     275     388     6Ø2     886    13Ø1
  155Ø    1657    1736    1691    1619    1634    16Ø1    1576    154Ø    1545
  151Ø    15Ø7    1425    1272    1Ø78     617     125       9       2       Ø
     Ø       1       1       Ø       Ø       1       Ø       Ø       Ø       1
     Ø       1       Ø       Ø       Ø       Ø       Ø       Ø       1
```

```
   299      1    299       Ø    22Ø6       Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG54          EXPERIMENT: EU/SR/S/SI
NAME......: BOE/SCHE             DATE/TIME.: 27: 8:82 / 1Ø:45:55
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 6Ø
ANAL.DOSE.: 2ØE-6 C              ANAL.ENERG: 2 MEV
THETA.....: 165 DEG              MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X        NOTE2.....: 1ØØØ CH/1Ø V
          S          EU          SR
      Ø.Ø        Ø.413     Ø.51Ø     Ø.Ø76     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.377D+17     Ø.434     Ø.535     Ø.Ø31     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.756D+17     Ø.459     Ø.517     Ø.Ø23     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.114D+18     Ø.491     Ø.492     Ø.Ø17     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.152D+18     Ø.5ØØ     Ø.462     Ø.Ø37     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.173D+18     Ø.5Ø2     Ø.464     Ø.Ø34     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.193D+18     Ø.538     Ø.434     Ø.Ø29     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.214D+18     Ø.538     Ø.438     Ø.Ø25     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.235D+18     Ø.519     Ø.451     Ø.Ø3Ø     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.256D+18     Ø.534     Ø.431     Ø.Ø35     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.277D+18     Ø.536     Ø.412     Ø.Ø52     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.298D+18     Ø.53Ø     Ø.369     Ø.1Ø2     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.319D+18     Ø.527     Ø.284     Ø.189     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.341D+18     Ø.518     Ø.185     Ø.297     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.363D+18     Ø.513     Ø.117     Ø.37Ø     Ø.Ø       Ø.Ø       Ø.Ø
   Ø.385D+18     Ø.5Ø9     Ø.Ø74     Ø.417     Ø.Ø       Ø.Ø       Ø.Ø
```

The output this time includes two warnings: The spectrum has now been evaluated to such depths from which the S-signal may now be superposed on Si-signals from shallower depths, and the Eu-signal may be superposed on the Sr-signal.

Although this has partly been avoided by evaluating the surface layer from another spectrum (see b. above), and slightly larger depths with the independent knowledge that Si is only found even deeper (see c. above), the evaluation of S-signals from channel 153 and below is not possible (these channels were already evaluated as Si-signals). Correspondingly, signals from channels 223-243 clearly originate from scattering on Sr, and thus may not be evaluated as Eu-signals.

In conclusion we may only believe in the derived targetcomposition up to a depth of $\sim 7.24 \cdot 10^{17}$ atoms/cm^2. Figures 11a-11d show the results.

3 consecutive runs like these of course require relatively long CPU-time, in the present case a total of $\sim$ 8 seconds.

```
SCATTERING ANGLE =   165.Ø , INC.ANGLE =    6Ø.Ø AND EXIT-ANGLE =    61.1 DEGREES

INCIDENT ENERGY =   2ØØØ. KEV.    6.391 KEV/CHANNEL,  AND ENERGY =   41.172 IN CHANNEL Ø

STOP EVALUATION WHEN EBEAM<   1ØØØ. KEV, OR WHEN CHANNELS BELOW CH. 13Ø ARE REQUESTED

 1 SPECTRA ARE EVALUATED WITH THIS INPUT

PROJECTILE HAS MASS =      4.ØØ2, AND Z =  2
 ENERGY-SCALING FACTOR     1.ØØØ

            TARGET-ELEMENTS
            ---------------

NAME    MASS         Z                                   COEFFICIENTS

 S       32.Ø6Ø      16      Ø.14Ø2D+Ø1    Ø.6791D+ØØ    Ø.5898D+Ø2    Ø.3528D+Ø1    Ø.3211D+Ø1
EU      152.ØØØ      63      Ø.1422D+Ø2    Ø.363ØD+ØØ    Ø.2284D+Ø3    Ø.7Ø24D+Ø1    Ø.1Ø16D+Ø1
SR       87.63Ø      38      Ø.7126D+Ø1    Ø.48Ø4D+ØØ    Ø.1193D+Ø3    Ø.5784D+Ø1    Ø.2454D+Ø1
SI       28.Ø6Ø      14      Ø.21ØØD+Ø1    Ø.65ØØD+ØØ    Ø.4934D+Ø2    Ø.1788D+Ø1    Ø.4133D+Ø1

                SPECTRUM NO.  1

   299      1    299      Ø    22Ø6      Ø       Ø       Ø       1
AMOS-FI-SG: BMSD5.SEG54          EXPERIMENT: EU/SR/S/SI
NAME.....: BOE/SCHE              DATE/TIME.: 27: 8:82 / 1Ø:45:55
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 6Ø
ANAL.DOSE.: 2ØE-6 C              ANAL.ENERG: 2 MEV
THETA.....: 165 DEG              MATERIAL..: EU-S/SR-S/SI
TARGETPOS.: 39 MM                LOGBOOK...: RBS VI/175
NOTE1.....: H.V.GAIN=256X        NOTE2.....: 1ØØØ CH/1Ø V
```

0.	663.	2206.	1820.	1620.	1533.	1356.	1251.	1151.	1045.
1004.	1014.	990.	941.	921.	836.	851.	851.	775.	775.
730.	750.	739.	692.	719.	687.	717.	636.	643.	663.
643.	665.	596.	607.	624.	573.	579.	568.	552.	592.
518.	565.	577.	581.	527.	518.	522.	516.	488.	526.
538.	494.	519.	476.	520.	497.	493.	533.	481.	554.
506.	492.	533.	490.	433.	486.	475.	465.	492.	468.
478.	453.	465.	517.	476.	450.	478.	454.	435.	429.
448.	418.	478.	460.	426.	446.	399.	424.	413.	415.
415.	430.	397.	414.	402.	443.	379.	427.	404.	466.
399.	416.	453.	359.	429.	415.	380.	372.	389.	379.
414.	390.	387.	400.	362.	381.	360.	380.	362.	342.
323.	343.	367.	336.	334.	339.	326.	359.	329.	351.
372.	349.	361.	382.	338.	316.	333.	351.	370.	409.
408.	434.	388.	354.	270.	271.	159.	100.	73.	28.
18.	13.	14.	14.	25.	16.	23.	26.	47.	85.
123.	140.	180.	147.	157.	155.	156.	151.	146.	145.
143.	144.	145.	125.	146.	129.	105.	134.	134.	117.
121.	128.	102.	82.	39.	19.	11.	7.	17.	8.
11.	7.	7.	8.	10.	9.	7.	3.	10.	5.
6.	5.	8.	10.	10.	11.	7.	9.	8.	10.
11.	7.	17.	16.	14.	12.	16.	15.	12.	22.
26.	34.	23.	36.	55.	62.	136.	226.	348.	554.
694.	745.	819.	794.	792.	721.	630.	505.	321.	173.
85.	53.	46.	32.	39.	42.	47.	47.	53.	65.
83.	112.	126.	168.	176.	275.	388.	602.	886.	1301.
1550.	1657.	1736.	1691.	1619.	1634.	1601.	1576.	1540.	1545.
1510.	1507.	1425.	1272.	1078.	617.	125.	9.	2.	0.
0.	1.	1.	0.	0.	1.	0.	0.	0.	1.
0.	1.	0.	0.	0.	0.	0.	0.	1.	

DEPTH	STOCHIOMETRIC COEFFICIENTS,UNCERTAINTIES						CHANNELS						Q
TOMS/CM2	S	EU	SR	SI			S	EU	SR	SI			
0.0	.413	.510	.076	.0	.0	.0							
0.377D+17	.434	.535	.031	.0	.0	.0							
0.756D+17	.459	.517	.023	.0	.0	.0							
0.114D+18	.491	.492	.017	.0	.0	.0							
0.152D+18	.500	.462	.037	.0	.0	.0							
0.173D+18	.502	.464	.034	.0	.0	.0							
0.193D+18	.538	.434	.029	.0	.0	.0							
0.214D+18	.538	.438	.025	.0	.0	.0							
0.235D+18	.519	.451	.030	.0	.0	.0							
0.256D+18	.534	.431	.035	.0	.0	.0							
0.277D+18	.536	.412	.052	.0	.0	.0							
0.298D+18	.530	.369	.102	.0	.0	.0							
0.319D+18	.527	.284	.189	.0	.0	.0							
0.341D+18	.518	.185	.297	.0	.0	.0							
0.363D+18	.513	.117	.370	.0	.0	.0							
0.385D+18	.509	.074	.417	.0	.0	.0							
0.407D+18	.470,.04	.047,.00	.427,.02	.055,.01	.0 ,.0	.0 ,.0	166.	256.	235.	153.	0.	0.	0.194D+11
0.431D+18	.476,.04	.035,.00	.437,.02	.052,.01	.0 ,.0	.0 ,.0	165.	254.	234.	152.	0.	0.	0.193D+11
0.456D+18	.452,.04	.029,.00	.449,.02	.070,.02	.0 ,.0	.0 ,.0	164.	253.	233.	151.	0.	0.	0.193D+11
0.480D+18	.497,.04	.022,.00	.380,.01	.101,.02	.0 ,.0	.0 ,.0	163.	252.	232.	150.	0.	0.	0.199D+11
0.506D+18	.381,.03	.016,.00	.342,.01	.260,.03	.0 ,.0	.0 ,.0	162.	251.	231.	149.	0.	0.	0.195D+11
0.532D+18	.339,.03	.013,.00	.273,.01	.376,.04	.0 ,.0	.0 ,.0	161.	250.	230.	148.	0.	0.	0.178D+11
0.560D+18	.224,.03	.010,.00	.165,.01	.600,.05	.0 ,.0	.0 ,.0	160.	249.	229.	147.	0.	0.	0.165D+11
0.590D+18	.098,.01	.007,.00	.082,.01	.813,.05	.0 ,.0	.0 ,.0	159.	248.	228.	146.	0.	0.	0.191D+11
0.623D+18	.062,.01	.008,.00	.048,.00	.883,.05	.0 ,.0	.0 ,.0	158.	247.	227.	145.	0.	0.	0.173D+11
0.656D+18	.042,.01	.005,.00	.021,.00	.931,.05	.0 ,.0	.0 ,.0	157.	246.	226.	144.	0.	0.	0.207D+11
0.690D+18	.034,.01	.004,.00	.015,.00	.946,.05	.0 ,.0	.0 ,.0	156.	245.	224.	143.	0.	0.	0.222D+11
0.724D+18	.036,.01	.004,.00	.009,.00	.951,.05	.0 ,.0	.0 ,.0	155.	244.	223.	142.	0.	0.	0.241D+11
0.758D+18	.025,.01	.006,.00	.010,.00	.959,.05	.0 ,.0	.0 ,.0	154.	242.	222.	141.	0.	0.	0.227D+11
0.793D+18	.025,.01	.009,.00	.009,.00	.957,.05	.0 ,.0	.0 ,.0	153.	241.	221.	140.	0.	0.	0.224D+11
0.827D+18	.030,.01	.019,.00	.008,.00	.943,.05	.0 ,.0	.0 ,.0	152.	240.	220.	139.	0.	0.	0.209D+11
0.861D+18	.046,.01	.039,.00	.005,.00	.910,.05	.0 ,.0	.0 ,.0	151.	239.	219.	138.	0.	0.	0.209D+11
0.894D+18	.099,.01	.064,.00	.005,.00	.832,.05	.0 ,.0	.0 ,.0	149.	238.	218.	137.	0.	0.	0.222D+11
0.926D+18	.158,.02	.076,.00	.005,.00	.760,.04	.0 ,.0	.0 ,.0	148.	237.	217.	136.	0.	0.	0.243D+11
0.957D+18	.209,.02	.075,.00	.003,.00	.712,.04	.0 ,.0	.0 ,.0	147.	236.	216.	135.	0.	0.	0.283D+11
0.989D+18	.298,.02	.068,.00	.003,.00	.631,.03	.0 ,.0	.0 ,.0	146.	235.	215.	134.	0.	0.	0.338D+11
0.102D+19	.341,.02	.068,.00	.004,.00	.587,.03	.0 ,.0	.0 ,.0	145.	234.	214.	133.	0.	0.	0.346D+11
0.105D+19	.388,.02	.061,.00	.003,.00	.549,.03	.0 ,.0	.0 ,.0	144.	233.	213.	132.	0.	0.	0.371D+11
0.108D+19	.422,.02	.053,.00	.002,.00	.523,.03	.0 ,.0	.0 ,.0	143.	231.	211.	131.	0.	0.	0.388D+11

I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*

NG! S-SIGNAL EVALUATED SO DEEP THAT IT MAY RUN INTO SI-SIGNAL!!

I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*

NG! EU-SIGNAL EVALUATED SO DEEP THAT IT MAY RUN INTO SR-SIGNAL!!

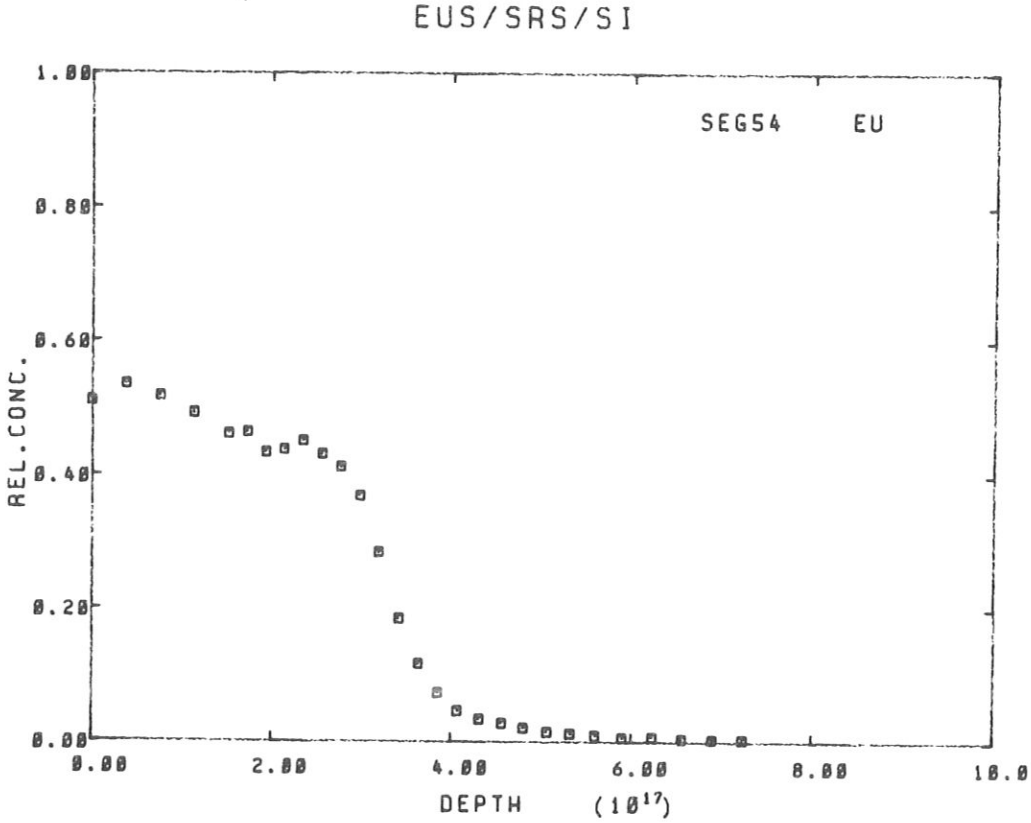


Fig. 11a: Plot of SQUEAKIE - output resulting from evaluation of the spectra in Figs. 9 and 10. Original SQUEAKIE-version. Relative concentration vs. depth of Eu.

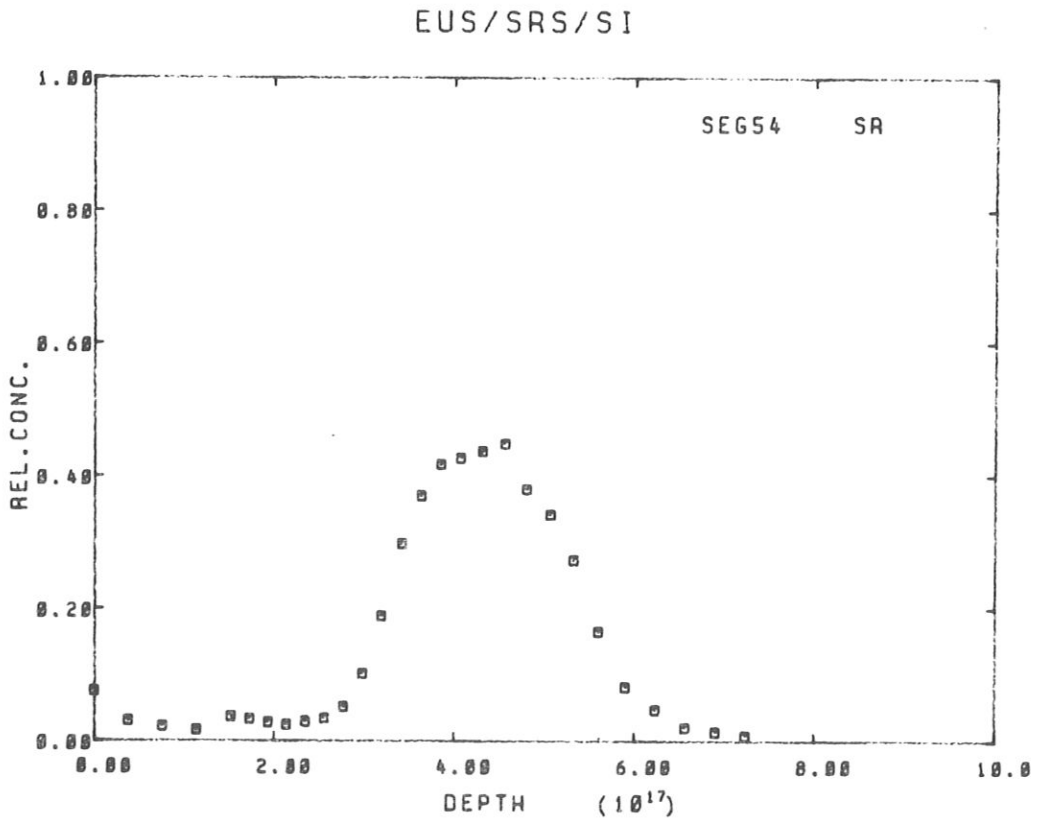


Fig. 11b: Relative concentration vs. depth of Sr

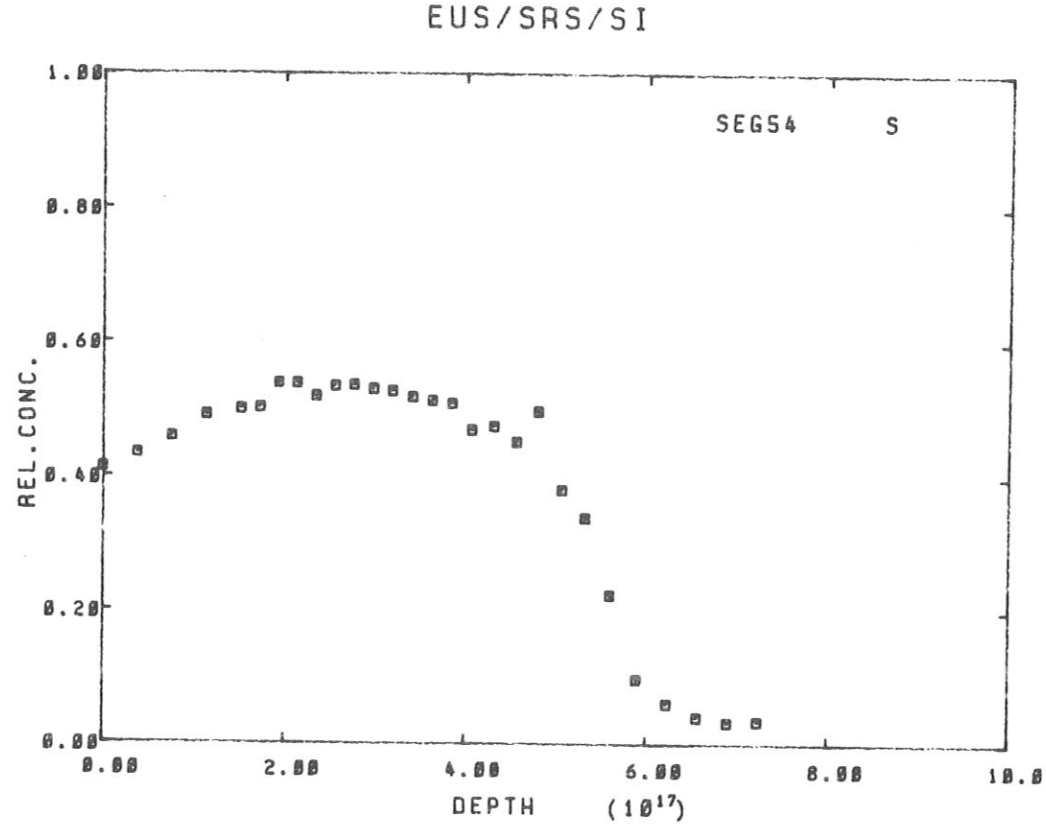


Fig. 11c: Relative concentration vs. depth of S.

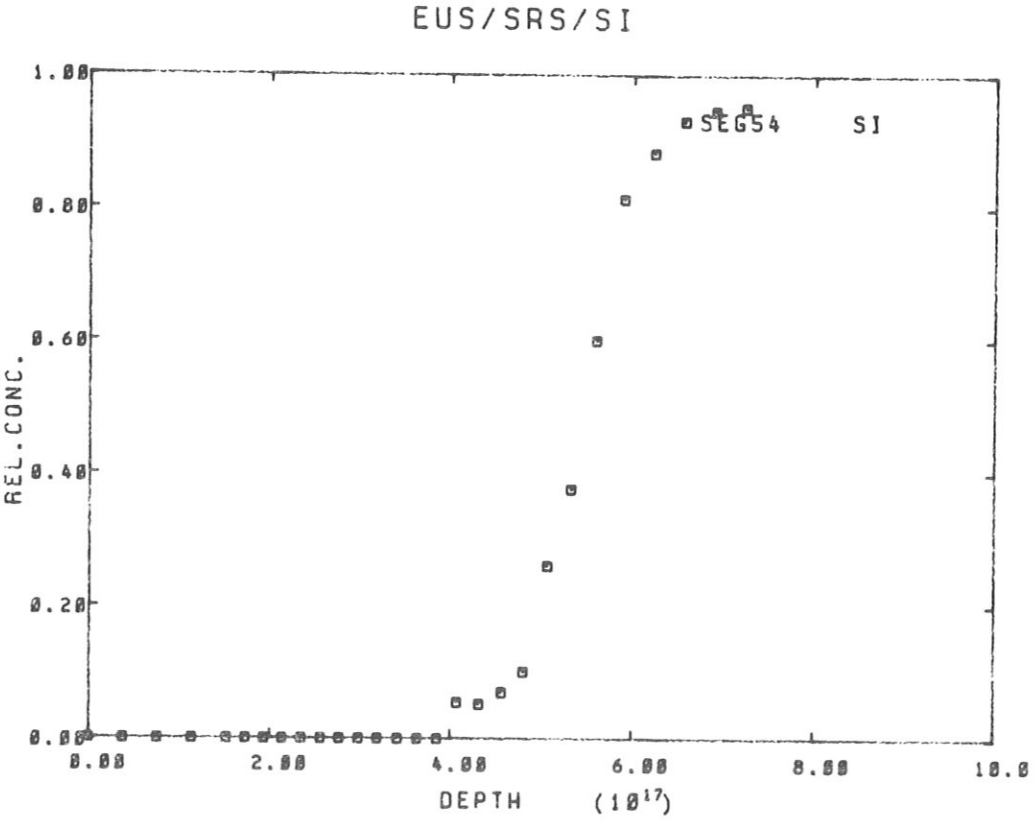


Fig. 11d: Relative concentration vs. depth of Si.

3. The final example demonstrates the use of the alternative version of the program:

The spectrum is the same as used in the first example, but this time we include all three target elements (Eu, S, and Si) in the evaluation. We can therefore also go to much larger depths, but we have to assume that no Eu- or S-signals are superposed on the Si-signal. After a study of the spectrum we then specify the Eu-signals to be confined to the interval between ch1(Eu) = 199 and ch2(Eu) = 230. Correspondingly we let ch1(S) = 128 and ch2(S) = 161, and assume that all Si-signals fall in or below channel number 127. The evaluation in the present case is terminated when the Si-signal falls below channel 90.

The necessary input was of course the spectrum (as above), preceded by the set of parameters:

```
170.0      60.0      60.5
2000.      7.6830    +55.000
                1 2 0
 3
 1    289
4.0016          2    1.0
32.06          16    S          128          161
1.402       E+0 6.791       E-1 5.898       E+1 3.528       E+0 3.211       E+0
152.0          63    EU         199          230
1.422       E+1 3.63        E-1 2.284       E+2 7.024       E+0 1.016       E+0
28.06          14    SI          90          127
2.1         E+0 6.5         E-1 4.934       E+1 1.788       E+0 4.133       E+0
```

The output is on the same form as before, except that also the element markers are given.

```
SCATTERING ANGLE =   170.0 , INC.ANGLE =    60.0 AND EXIT-ANGLE =    60.5 DEGREES

INCIDENT ENERGY =   2000. KEV,    7.683 KEV/CHANNEL,  AND ENERGY =   55.000 IN CHANNEL 0

 1 SPECTRA ARE EVALUATED WITH THIS INPUT

PROJECTILE HAS MASS =      4.002, AND Z =  2
 ENERGY-SCALING FACTOR      1.000

                TARGET-ELEMENTS
                ---------------

NAME    MASS   Z   INTERVAL                          COEFFICIENTS

 S     32.06   16   128  161   0.1402D+01  0.6791D+00  0.5898D+02  0.3528D+01  0.321
EU    152.00   63   199  230   0.1422D+02  0.3630D+00  0.2284D+03  0.7024D+01  0.181
SI     28.06   14    90  127   0.2100D+01  0.6500D+00  0.4934D+02  0.1788D+01  0.413
```

SPECTRUM NO. 1

```
   29Ø   44Ø1   469Ø   11Ø4   68ØØ      Ø      Ø      Ø      1
AMOS-FI-SG: BMSD4.SEG57          EXPERIMENT: EU-S/SI ANALYSE
NAME.....: BOR/SCHE              DATE/TIME.: 27: 7:82 / 16:28:21
IMPL.IONS.:                      IMPL.ENERG:
IMPL.FLNCE:                      ANALYSIS..: RBS
ANAL.IONS.: 4HE                  ALPHA.....: 6ØDEG
ANAL.DOSE.: 1.25E-7 C            ANAL.ENERG: 2 MEV
THETA.....: 17Ø DEG              MATERIAL..: 111Ø A EUS/SI
TARGETPOS.: 29 MM                LOGBOOK...: BMS II/23
NOTE1.....: 5ØØ CH./1Ø V         NOTE2.....: HV 256X
 3859.   3673.   1138.   1788.    3891.   6828.   6888.   6354.   5533.   4955.
 4281.   3937.   3685.   3311.    3877.   2865.   2685.   2597.   2273.   2203.
 2151.   2878.   2872.   1881.    1927.   1863.   1767.   1755.   1679.   1584.
 1615.   1594.   1525.   1475.    1499.   1464.   1438.   1345.   1354.   1354.
 1343.   1344.   1288.   1293.    1318.   1224.   1235.   1278.   1191.   1261.
 1283.   1171.   1171.   1177.    1142.   1285.   1146.   1156.   1142.   1146.
 1118.   1131.   1895.   1843.    1868.   1868.   1884.   1837.   1877.   1884.
 1812.   1868.   1825.   1883.    1844.   1811.    992.   1869.   1829.    976.
 1822.    959.   1885.   1816.     981.    986.    932.    945.    948.    978.
  879.    939.    918.    978.     956.    959.    916.    985.    868.    939.
  988.    897.    894.    849.     921.    812.    987.    949.    984.    831.
  947.    848.    928.    923.     926.    894.    827.    759.    652.    634.
  478.    488.    348.    228.     125.    188.     64.     81.    186.    112.
  128.    173.    282.    231.     295.    297.    331.    338.    338.    383.
  356.    355.    321.    336.     385.    338.    346.    347.    314.    289.
  182.    134.     59.     28.      28.     34.     24.     21.     22.     21.
   15.     21.     15.     18.      13.     24.     15.     22.     13.     19.
   14.     17.     19.     17.      23.     28.     21.     17.     13.     15.
   16.     21.     21.     17.      19.     26.     19.     18.     19.     29.
   28.     38.     35.     41.      32.     44.     42.     76.    121.    188.
  389.    558.    842.   1219.    1638.   2216.   2749.   3398.   3832.   4348.
 4495.   4676.   4598.   4699.    4748.   4585.   4787.   4668.   4686.   4586.
 4696.   4685.   4577.   4636.    4299.   3715.   2698.   1364.    379.     77.
    8.      8.      4.      7.       6.      Ø.      2.      5.      2.      3.
    4.      1.      5.      3.       1.      5.      2.      2.      1.      1.
    2.      Ø.      1.      Ø.       2.      3.      Ø.      1.      3.      3.
    Ø.      1.      3.      1.       3.      2.      4.      2.      Ø.      1.
    1.      2.      Ø.      1.       1.      2.      2.      1.      Ø.      1.
    2.      2.      Ø.      2.       1.      1.      1.      Ø.      Ø.
```

DEPTH	STOCHIOMETRIC COEFFICIENTS,UNCERTAINTIES										CHANNELS						Q
ATOMS/CM2	S		EU		SI						S	EU	SI				
Ø	.538,.Ø4		.462,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	151.	227.	148.	Ø.	Ø.	Ø.	Ø.189D+11
25ØD+17	.546,.Ø3		.454,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	158.	226.	139.	Ø.	Ø.	Ø.	Ø.285D+11
581D+17	.525,.Ø3		.475,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	149.	225.	138.	Ø.	Ø.	Ø.	Ø.335D+11
747D+17	.523,.Ø3		.477,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	148.	224.	137.	Ø.	Ø.	Ø.	Ø.367D+11
993D+17	.525,.Ø3		.475,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	147.	223.	136.	Ø.	Ø.	Ø.	Ø.373D+11
124D+18	.518,.Ø3		.482,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	146.	222.	136.	Ø.	Ø.	Ø.	Ø.368D+11
148D+18	.499,.Ø3		.581,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	146.	221.	135.	Ø.	Ø.	Ø.	Ø.364D+11
172D+18	.582,.Ø3		.498,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	145.	228.	134.	Ø.	Ø.	Ø.	Ø.361D+11
196D+18	.513,.Ø3		.487,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	144.	219.	133.	Ø.	Ø.	Ø.	Ø.364D+11
221D+18	.589,.Ø3		.491,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	143.	218.	132.	Ø.	Ø.	Ø.	Ø.365D+11
245D+18	.526,.Ø3		.474,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	142.	217.	131.	Ø.	Ø.	Ø.	Ø.376D+11
269D+18	.529,.Ø3		.471,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	141.	216.	138.	Ø.	Ø.	Ø.	Ø.367D+11
293D+18	.487,.Ø3		.513,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	148.	215.	129.	Ø.	Ø.	Ø.	Ø.354D+11
317D+18	.584,.Ø3		.496,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	139.	214.	128.	Ø.	Ø.	Ø.	Ø.364D+11
341D+18	.476,.Ø3		.447,.Ø1		.Ø76,.Ø1		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	138.	213.	127.	Ø.	Ø.	Ø.	Ø.388D+11
368D+18	.435,.Ø2		.417,.Ø1		.149,.Ø2		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	137.	212.	126.	Ø.	Ø.	Ø.	Ø.399D+11
396D+18	.396,.Ø2		.485,.Ø1		.199,.Ø2		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	136.	211.	125.	Ø.	Ø.	Ø.	Ø.392D+11
425D+18	.351,.Ø2		.352,.Ø1		.297,.Ø2		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	135.	218.	124.	Ø.	Ø.	Ø.	Ø.414D+11
454D+18	.267,.Ø2		.291,.ØØ		.442,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	134.	289.	123.	Ø.	Ø.	Ø.	Ø.411D+11
485D+18	.222,.Ø2		.241,.ØØ		.537,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	133.	288.	122.	Ø.	Ø.	Ø.	Ø.486D+11
518D+18	.188,.Ø1		.188,.ØØ		.624,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	132.	287.	121.	Ø.	Ø.	Ø.	Ø.398D+11
552D+18	.128,.Ø1		.132,.ØØ		.748,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	131.	286.	128.	Ø.	Ø.	Ø.	Ø.488D+11
588D+18	.187,.Ø1		.892,.ØØ		.881,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	138.	285.	119.	Ø.	Ø.	Ø.	Ø.396D+11
625D+18	.895,.Ø1		.861,.ØØ		.844,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	129.	283.	118.	Ø.	Ø.	Ø.	Ø.485D+11
664D+18	.869,.Ø1		.838,.ØØ		.893,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	128.	282.	117.	Ø.	Ø.	Ø.	Ø.414D+11
784D+18	.881,.ØØ		.822,.ØØ		.977,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	127.	281.	116.	Ø.	Ø.	Ø.	Ø.488D+11
745D+19	.Ø	,.Ø	.812,.ØØ		.988,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	126.	288.	115.	Ø.	Ø.	Ø.	Ø.418D+11
785D+18	.Ø	,.Ø	.887,.ØØ		.993,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	125.	199.	114.	Ø.	Ø.	Ø.	Ø.418D+11
826D+18	.Ø	,.Ø	.Ø	,.Ø	****,.Ø3		.Ø	,.Ø	.Ø	,.Ø	.Ø	,.Ø	124.	198.	113.	Ø.	Ø.	Ø.	Ø.481D+11

0.868D+18	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	123.	197.	112.	0.	0.	0.	0.379D+11
0.909D+18	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	122.	196.	111.	0.	0.	0.	0.396D+11
0.950D+18	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	121.	195.	110.	0.	0.	0.	0.377D+11
0.991D+18	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	120.	194.	109.	0.	0.	0.	0.380D+11
0.103D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	119.	193.	108.	0.	0.	0.	0.402D+11
0.107D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	118.	192.	107.	0.	0.	0.	0.396D+11
0.111D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	117.	191.	106.	0.	0.	0.	0.363D+11
0.115D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	116.	190.	105.	0.	0.	0.	0.378D+11
0.119D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	115.	188.	104.	0.	0.	0.	0.373D+11
0.124D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	114.	187.	103.	0.	0.	0.	0.375D+11
0.128D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	113.	186.	102.	0.	0.	0.	0.381D+11
0.132D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	112.	185.	101.	0.	0.	0.	0.382D+11
0.136D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	111.	184.	100.	0.	0.	0.	0.392D+11
0.140D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	110.	183.	99.	0.	0.	0.	0.375D+11
0.144D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	109.	182.	98.	0.	0.	0.	0.375D+11
0.148D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	108.	181.	97.	0.	0.	0.	0.384D+11
0.152D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	107.	180.	96.	0.	0.	0.	0.397D+11
0.156D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	106.	179.	95.	0.	0.	0.	0.401D+11
0.160D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	105.	178.	94.	0.	0.	0.	0.404D+11
0.164D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	104.	177.	93.	0.	0.	0.	0.388D+11
0.167D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	103.	176.	92.	0.	0.	0.	0.387D+11
0.171D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	102.	175.	91.	0.	0.	0.	0.373D+11
0.175D+19	.0	,.0	.0	,.0	****,.03	.0	,.0	.0	,.0	.0	,.0	101.	174.	90.	0.	0.	0.	0.389D+11
0.179D+19	.0	,.0	.0	,.0	****,.06	.0	,.0	.0	,.0	.0	,.0	100.	172.	89.	0.	0.	0.	0.136D+11

I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*I*

WARNING! S-SIGNAL EVALUATED SO DEEP THAT IT MAY RUN INTO SI-SIGNAL!!

DEPTH — CONTENTS (ATOMS/CM**2) INTEGRATED FROM SURFACE

FROM ENERGYLOSS I FROM SCATTERING(DIVIDE BY DOSIS*SOLID-A

MOLEC./CM2	S	EU	SI				S	EU	SI
.0	.0	.0	.0	.0	.0	.0	.205D+27	.131D+27	.0
.250D+17	.135D+17	.115D+17	.0	.0	.0	.0	.484D+27	.391D+27	.0
.501D+17	.271D+17	.229D+17	.0	.0	.0	.0	.925D+27	.746D+27	.0
.747D+17	.401D+17	.347D+17	.0	.0	.0	.0	.140D+28	.116D+28	.0
.993D+17	.529D+17	.464D+17	.0	.0	.0	.0	.193D+28	.160D+28	.0
.124D+18	.658D+17	.581D+17	.0	.0	.0	.0	.245D+28	.203D+28	.0
.148D+18	.785D+17	.698D+17	.0	.0	.0	.0	.295D+28	.247D+28	.0
.172D+18	.905D+17	.819D+17	.0	.0	.0	.0	.340D+28	.291D+28	.0
.196D+18	.103D+18	.939D+17	.0	.0	.0	.0	.390D+28	.334D+28	.0
.221D+18	.115D+18	.106D+18	.0	.0	.0	.0	.438D+28	.377D+28	.0
.245D+18	.127D+18	.117D+18	.0	.0	.0	.0	.491D+28	.420D+28	.0
.269D+18	.140D+18	.129D+18	.0	.0	.0	.0	.543D+28	.464D+28	.0
.293D+19	.153D+18	.140D+18	.0	.0	.0	.0	.587D+28	.505D+28	.0
.317D+18	.164D+18	.153D+18	.0	.0	.0	.0	.636D+28	.549D+28	.0
.341D+18	.177D+18	.164D+18	.0	.0	.0	.0	.634D+28	.592D+28	.0
.368D+18	.190D+18	.177D+18	.209D+16	.0	.0	.0	.684D+28	.633D+28	.126D+27
.396D+18	.202D+18	.188D+18	.625D+16	.0	.0	.0	.731D+28	.676D+28	.322D+27
.425D+18	.213D+18	.200D+18	.119D+17	.0	.0	.0	.774D+28	.716D+28	.566D+27
.454D+18	.223D+18	.210D+18	.206D+17	.0	.0	.0	.816D+28	.755D+28	.101D+28
.485D+18	.232D+18	.219D+18	.344D+17	.0	.0	.0	.848D+28	.820D+28	.167D+28
.518D+18	.239D+18	.227D+18	.518D+17	.0	.0	.0	.876D+28	.844D+28	.244D+28
.552D+18	.245D+18	.233D+18	.731D+17	.0	.0	.0	.900D+28	.863D+28	.335D+28
.588D+18	.250D+18	.238D+18	.998D+17	.0	.0	.0	.917D+28	.876D+28	.457D+28
.625D+18	.254D+18	.242D+18	.130D+18	.0	.0	.0	.931D+28	.885D+28	.582D+28
.664D+18	.258D+18	.244D+18	.163D+18	.0	.0	.0	.945D+28	.891D+28	.727D+28
.704D+18	.260D+18	.246D+18	.198D+18	.0	.0	.0	.954D+28	.894D+28	.885D+28
.745D+18	.260D+18	.246D+18	.238D+18	.0	.0	.0	.954D+28	.895D+28	.105D+29
.785D+18	.260D+18	.247D+18	.278D+18	.0	.0	.0	.954D+28	.895D+28	.123D+29
.826D+18	.260D+18	.247D+18	.319D+18	.0	.0	.0	.954D+28	.894D+28	.140D+29
.868D+18	.260D+18	.247D+18	.360D+18	.0	.0	.0	.954D+28	.894D+28	.158D+29
.909D+18	.260D+18	.247D+18	.401D+18	.0	.0	.0	.954D+28	.894D+28	.173D+29
.950D+18	.260D+18	.247D+18	.443D+18	.0	.0	.0	.954D+28	.894D+28	.191D+29
.991D+18	.260D+18	.247D+18	.484D+18	.0	.0	.0	.954D+28	.894D+28	.206D+29
.103D+19	.260D+18	.247D+18	.525D+18	.0	.0	.0	.954D+28	.894D+28	.223D+29
.107D+19	.260D+18	.247D+18	.565D+18	.0	.0	.0	.954D+28	.894D+28	.241D+29
.111D+19	.260D+18	.247D+18	.606D+18	.0	.0	.0	.954D+28	.894D+28	.257D+29
.115D+19	.260D+18	.247D+18	.647D+18	.0	.0	.0	.954D+28	.894D+28	.272D+29
.119D+19	.260D+18	.247D+18	.687D+18	.0	.0	.0	.954D+28	.894D+28	.289D+29
.124D+19	.260D+18	.247D+18	.728D+18	.0	.0	.0	.954D+28	.894D+28	.304D+29
.128D+19	.260D+18	.247D+18	.768D+18	.0	.0	.0	.954D+28	.894D+28	.320D+29
.132D+19	.260D+18	.247D+18	.808D+18	.0	.0	.0	.954D+28	.894D+28	.336D+29
.136D+19	.260D+18	.247D+18	.849D+18	.0	.0	.0	.954D+28	.894D+28	.352D+29
.140D+19	.260D+18	.247D+18	.889D+18	.0	.0	.0	.954D+28	.894D+28	.369D+29
.144D+19	.260D+18	.247D+18	.929D+18	.0	.0	.0	.954D+28	.894D+28	.384D+29
.148D+19	.260D+18	.247D+18	.969D+18	.0	.0	.0	.954D+28	.894D+28	.400D+29
.152D+19	.260D+18	.247D+18	.101D+19	.0	.0	.0	.954D+28	.894D+28	.416D+29
.156D+19	.260D+18	.247D+18	.105D+19	.0	.0	.0	.954D+28	.894D+28	.433D+29
.160D+19	.260D+18	.247D+18	.109D+19	.0	.0	.0	.954D+28	.894D+28	.449D+29
.164D+19	.260D+18	.247D+18	.113D+19	.0	.0	.0	.954D+28	.894D+28	.466D+29
.167D+19	.260D+18	.247D+18	.117D+19	.0	.0	.0	.954D+28	.894D+28	.482D+29
.171D+19	.260D+18	.247D+18	.121D+19	.0	.0	.0	.954D+28	.894D+28	.498D+29
.175D+19	.260D+18	.247D+18	.125D+19	.0	.0	.0	.954D+28	.894D+28	.513D+29
.179D+19	.260D+18	.247D+18	.129D+19	.0	.0	.0	.954D+28	.894D+28	.530D+29
.183D+19	.260D+18	.247D+18	.132D+19	.0	.0	.0	.954D+28	.894D+28	.530D+29

In the tabulation of the stoichiometric coefficients vs. depth we see that the choice of these markers excludes the presence of S at depths larger than $7 \cdot 10^{17}$ atoms/cm^2, of Eu at depths larger than $8 \cdot 10^{17}$ atoms/cm^2, and of Si at depths smaller than $\sim 3.4 \cdot 10^{17}$ atoms/cm^2. We have no direct check of the validity of this, and correspondingly the table is followed by a warning.

Because of the element markers the calculated coefficient for Si must equal one at depths larger than $8 \cdot 10^{17}$ atoms/cm^2. On the printed output this appears as **** because of the corresponding FORMAT-statement (line no. 35500 in "STEP"), but on the output-segment it is written correctly. Figure 12 shows plots from this segment.

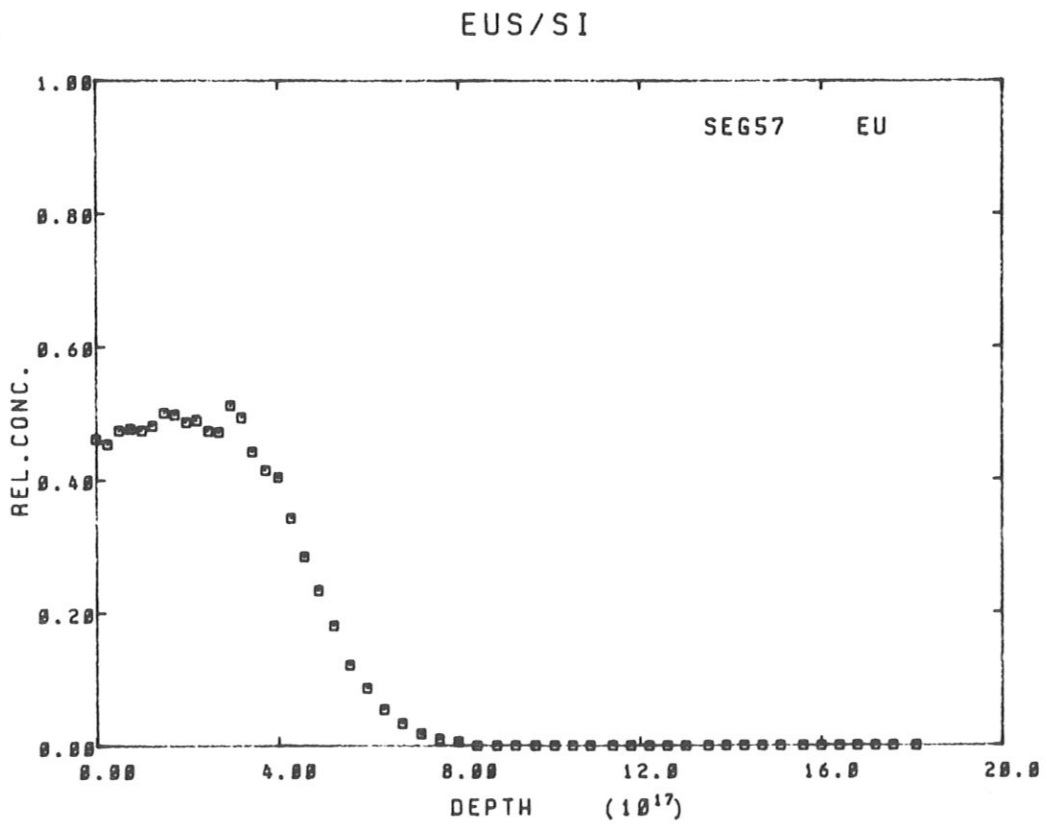


Fig. 12a: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig.6. Alternative SQUEAKIE-version. Relative concentration vs. depth of Eu.

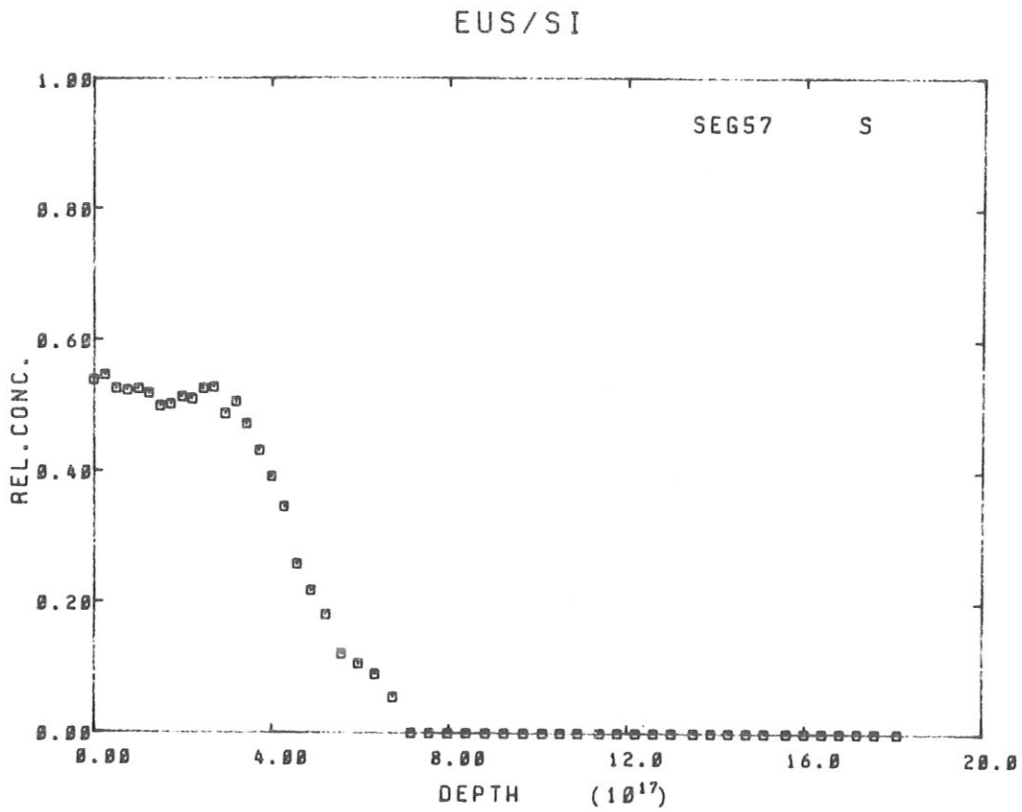


Fig. 12b: Relative concentration vs. depth of S.

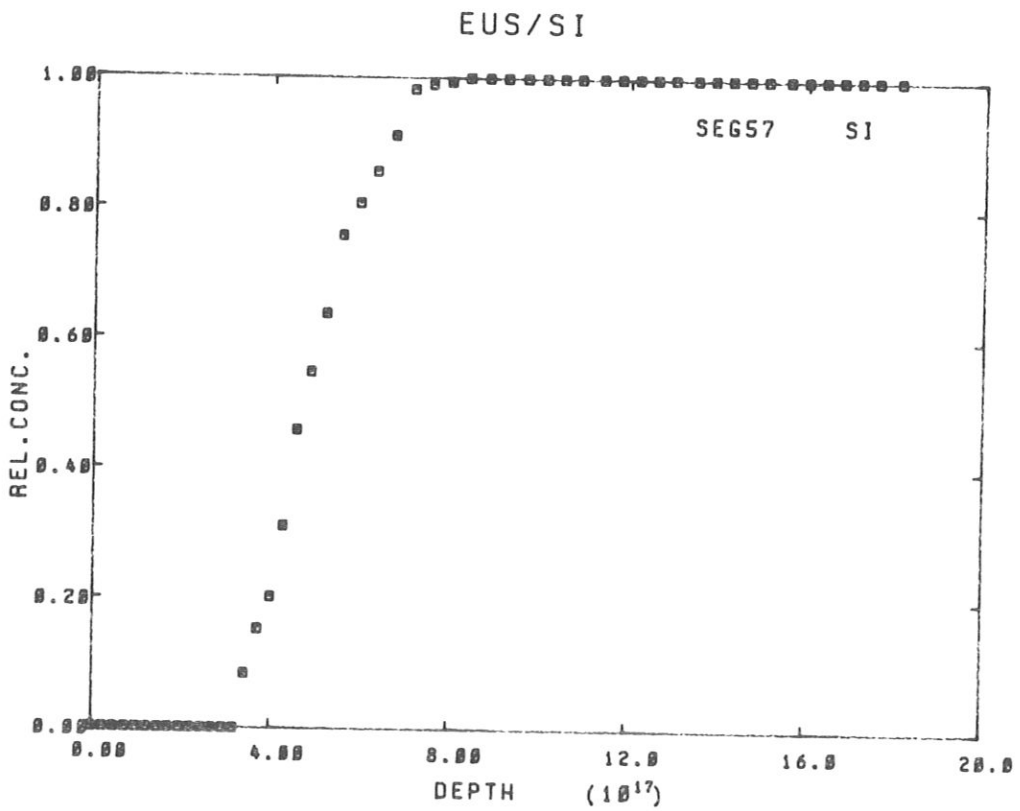


Fig. 12c: Relative concentration vs. depth of Si.

At those depths, where only one element is present, no inverse iteration and improved estimate of Q (Sect. 4.4) was performed. Instead the value Q was simply calculated from the experimental signal, i.e. from eqs. 2.1-2.4. It is seen that Q remains approximately constant up to more than $1.75 \cdot 10^{18}$ atoms/cm^2, and in good agreement with the 'iterated' values from shallower depths. S- or Eu-signals superposed on the Si-signal would result in larger Q-values than estimated from the inverse iteration, so we may conclude that such signals contribute less than $\sim$ 5 % of the evaluated Si-signal.

Using an average value of $3.8 \cdot 10^{10}$ for $N_{prim}\ \Delta\Omega$ we may again estimate the integrated contents from the scattering yields: The values $2.5 \cdot 10^{17}$ S-atoms/cm^2 and $2.35 \cdot 10^{17}$ Eu-atoms/cm^2 are in very good agreement with the results determined from the stoichiometry vs. depth.

6.6 Warnings

i) The present program should not be used by anyone who is not familiar at least with Sect. 2.1 and Chapter 3. Furthermore a study of Sect. 6.5 is recommended.

ii) The program may not always distinguish between signals from a light element near the surface or a heavy element at larger depth. After each run one should therefore check the printed output vs. the spectrum in order to ascertain that the various channels have been ascribed to the appropriate elements.

iii) If some targetelement (e.g. the substrate under a film) is not taken into account, one may at some depth evaluate only noise level signals (background). If none of the elemental signals are significant the resulting faulty stoichiometry may not be obvious. Besides from an inspection of the channel numbers (see above) also a study of the listed eigenvalues Q will reveal this: When Q falls by an order of magnitude or more, something is wrong.

iv) One should never accept negative stoichiometric coefficients, even if they are very small. The appearance of a negative coefficient indicates that the wrong eigenvector was found; i.e. the stoichiometry at this depth is probably very wrong. Such an error influences all results at larger depths, although perhaps. weakly.
This error was never encountered yet, except when deliberately provoked.

v) The most common input error has been the specification of the wrong number of channels in the spectrum. This usually causes a program interrupt (certainly if the results of previous spectra are included).

vi) Another common input error is the specification of target element data for fewer or more targetelements than given in Record # 4 (Sect. 6.3). This is also a terminal error.

7. TESTS

Two quite different types of tests are described below. One type is designed to ensure that the program functions correctly, i.e. that there are no programming errors. This of course is relevant when implementing the program on another computer, and may even partly be applied to other versions of the program.

The second type of tests has been performed by the authors in order to investigate precision, stability, speed etc. of the program. This is thus also partly a documentation of the applicability of the approach, as already described in Ref. 1.

7.1 Test of programming

Implementing the listed program on another computer, one is bound to experience malfunctions due to language modifications, available libraries, simple typing errors, etc. Most of these are easily identified, but errors may still remain which call for a closer examination. Below is listed a simple test-program, which may help to localize errors in the functions/subroutines.

The MAIN program as well as the subroutine STEP are best tested by repeating one of the examples listed in Section 6.5 (preferably examples 1 or 3).

```
C       *****
C       PROGRAM TEST
C      *****
C
C     TEST OF SUBROUTINES
C
        IMPLICIT REAL*8(A-H,O-S),INTEGER(I-N)
        COMMON/CALIB/THETA,ALFA,BETA,OFFS,DE1
        COMMON/COLL/A1,A(6),IZ1,IZ(6)
        DIMENSION AM(6,6),S(6),CF(5)
        N=4
        S(1)=4.Ø
        S(2)=2.Ø
        S(3)=2.5
         S(4)=3.Ø
        AM(1,1)=1.
        AM(1,2)=1.
        AM(1,3)=1.
        AM(1,4)=Ø.25
        AM(2,1)=2.
        AM(2,2)=Ø.5
        AM(2,3)=1.
        AM(2,4)=2.
        AM(3,1)=1.
        AM(3,2)=1.
        AM(3,3)=2.
        AM(3,4)=3.
        AM(4,1)=4.
        AM(4,2)=1.5
        AM(4,3)=1.
        AM(4,4)=4.5
        QØ=6.Ø
        CALL ITER(AM,S,QØ,N)
        WRITE(6,1ØØ)(S(I),I=1,N),QØ
 1ØØ    FORMAT(2X,7E12.3)
        EN= 1.ØD3
        IT=1
        A(IT)=152
        IZ(IT)=63
        THETA=165*3.14159/18Ø.
        A1=4.
        IZ1=2
        CR=CRSEC(EN,IT)
        WRITE(6,1Ø1)CR
 1Ø1    FORMAT(3X,'CROSS SECTION =',E12.4,' CM2',/)
        XK1=XK(IT)
        WRITE(6,1Ø2)XK1
 1Ø2    FORMAT(3X,'KINEMATIC FACTOR= ',E12.4,//)
        CF(1)=Ø.1422D+Ø2
        CF(2)=Ø.363ØD+ØØ
        CF(3)=Ø.2284D+Ø3
        CF(4)=Ø.7Ø24D+Ø1
        CF(5)=Ø.1Ø16D+Ø1
        FE=1.Ø
        STP=STPA(CF,FE,EN)
        WRITE(6,1Ø3)STP
 1Ø3    FORMAT(3X,'STOPPING POWER=',E12.4,' *1Ø**(-15) EV*CM2/ATOM',//)
        STOP
        END
```

Submission of this program together with the subroutine ITER and the functions XK, CRSEC and STPA should provide you with the result of an inverse iteration, as well as with the scattering cross-section ($d\sigma/d\Omega$), the kinematic factor K, and the stopping power S for 1 MeV $^4He^+$-ions incident on Eu and a scattering angle $\theta = 165^o$. The correct output is:

```
  Ø.25ØD+ØØ   Ø.5ØØD+ØØ   Ø.749D+ØØ   Ø.1ØØD+Ø1   Ø.7ØØD+Ø1
CROSS SECTION =  Ø.2114D-22 CM2

KINEMATIC FACTOR=   Ø.9Ø17D+ØØ

STOPPING POWER=  Ø.1296D+Ø3 *1Ø**(-15) EV*CM2/ATOM
```

Most difficult to find are errors in the subroutine ITER. If the output above shows a malfunction of ITER, or if the testprogram runs for longer than a few seconds (indicating a lack of convergence in ITER), you may therefore still need help to localize the error(s). In that case you simply run the testprogram again, but this time insert a few statements to print out various parameters at different stages in ITER:

Consider the listing of ITER in Sect. 5.7. Immediately before the statement labeled 300 the array AGEM should hold the values

-5	$7.452 \cdot 10^{28}$	$-1.636 \cdot 10^{78}$	$5.334 \cdot 10^{-21}$
2	-2.55	$1.987 \cdot 10^{28}$	$1.027 \cdot 10^{38}$
1	1.2	-2.892	$8.182 \cdot 10^{-79}$
4	0.575	1.057	0.876

If this is so, the error occurs in the iteration itself (below 300). During the first step of the iteration, the array S must contain (0.8, 0.7059, 1.195, -5.037) immediately after the statement labeled 200, and the array T should hold (0.7321, 2.452, 3.949, 5.037) after 210.

7.2 Test of program

i. The power of the present program depends largely on the swift convergence of the inverse iteration at each depth step (see Sect. 3.2). Let us therefore first test this:

The eigenvector problem

$$\begin{pmatrix} 1. & 1. & 1. & 0.25 \\ 2. & 0.5 & 1. & 2. \\ 1. & 1. & 2. & 3. \\ 4. & 1.5 & 1. & 4.5 \end{pmatrix} \underline{s}_r = Q\,\underline{s}_r \qquad (7.1)$$

has the solution $\underline{s}_r$ = (0.25, 0.5, 0.75, 1.) and the eigenvalue Q = 7. A very crude 'initial guess' is here $\underline{s}_{in}$ = (4, 2, 2.5, 3) and Q_o = 6 (this was used as a test in the previous section). Following the algorithm of Sect. 4.4, the iteration ran as indicated in the table below, leading to an excellent approximation $\underline{y}_k = (y_1, y_2, y_3, y_4)$ of $\underline{s}_r$ in 3-4 steps:

Iterated vector	y_1	y_2	y_3	y_4	'Iterated' Q
$\underline{y}_o$	1.33	0.667	0.833	1.	6.0
$\underline{y}_1$	0.1453	0.4868	0.784	1.	6.199
$\underline{y}_2$	0.2667	0.5011	0.7354	1.	7.054
$\underline{y}_3$	0.2478	0.5002	0.754	1.	6.995
$\underline{y}_4$	0.2502	0.4999	0.7491	1.	7.000

Table 1

This is only a 'mathematical' test of the subroutine ITER (Sect. 5.6); the present parameters will probably never occur in a physically relevant situation. Unlike for experimental spectra /1/ we may not even be sure that Eq. 7.1 does not have more eigenvectors with only positive, real coordinates. Nevertheless, in spite of an unusually

bad 'initial guess' we see a very swift convergence of the iteration, adjusting 'concentrations' by up to a factor of 4, and the eigenvalue by 17 %. Actually, even with the guess $Q_o = 4.0$ the iteration would converge to the same $\underline{y}_k$ within $\sim$ 40 steps, at the expense of only $\sim$ 0.07 seconds extra CPU-time.

ii. Quite thorough tests of the program itself were already described in Ref. 1. Further tests have now been performed, showing the individual effects of isotopes, system resolution, energy straggling and counting statistics.

The only way to fully determine the influence of the individual parameters is to test the program on synthesized spectra. For this purpose energy spectra were calculated /21, 8/, corresponding to Rutherford backscattering of $^4He^+$-ions from a target composed of 4 layers, each of constant stoichiometry:

1. layer : $C_{0.55}\ Mg_{0.25}\ Ti_{0.15}\ Bi_{0.05}$, $1 \cdot 10^{18}$ atoms/cm^2
2. layer : $C_{0.2}\ Mg_{0.1}\ Ti_{0.4}\ Bi_{0.3}$, $7.5 \cdot 10^{17}$ "
3. layer : $C_{0.05}\ Mg_{0.1}\ Ti_{0.7}\ Bi_{0.15}$, $7.5 \cdot 10^{17}$ "
4. layer : $C_{0.8}\ Ti_{0.2}$, $1 \cdot 10^{18}$ "

The "experimental" parameters were taken as E_o = 2 MeV, $N_{prim}\ \Delta\Omega = 10^{11}$ ions•sterad, $\theta = 161^o$, $\alpha = 19^o$, $\beta = 0^o$, ΔE_1 = 3.3 keV/channel, and an offset of 230 keV corresponding to channel Ø. The spectra were calculated in depthsteps of $1.1 \cdot 10^{16}$ atoms/cm^2.

a) As already seen previously /1/, the program yields the correct target composition quite accurately, unless the spectrum is somehow perturbed by isotope effects, resolution, statistics, etc.
Figure 13 shows the logarithmic plot of the ideal, synthesized spectrum.

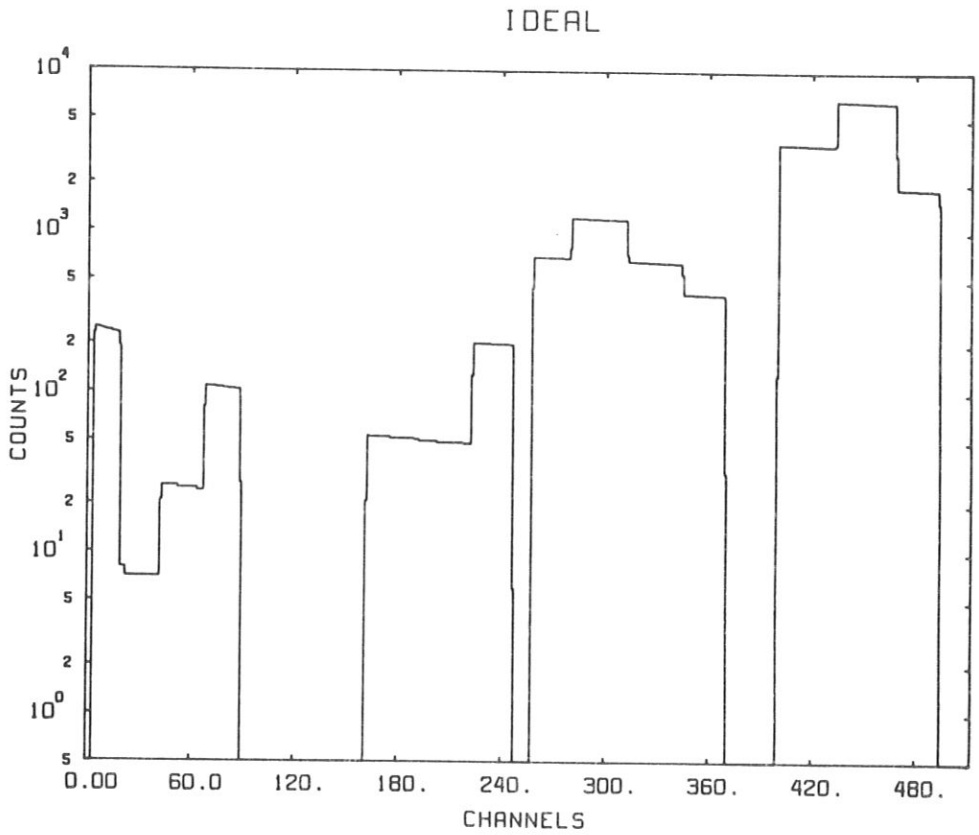


Fig. 13: Synthesized RBS-spectrum, ideal case (see text). Note logarithmic axis!

With this as input in SQUEAKIE we find the correct target composition vs. depth, except at the interfaces (see Fig. 14a). At surface/interfaces errors arise, both in the generated spectrum and in the evaluation with SQUEAKIE, because of the finite depthsteps used in both programs. These errors are reflected in a plot of the eigenvalue Q vs. depth (Fig. 14b).

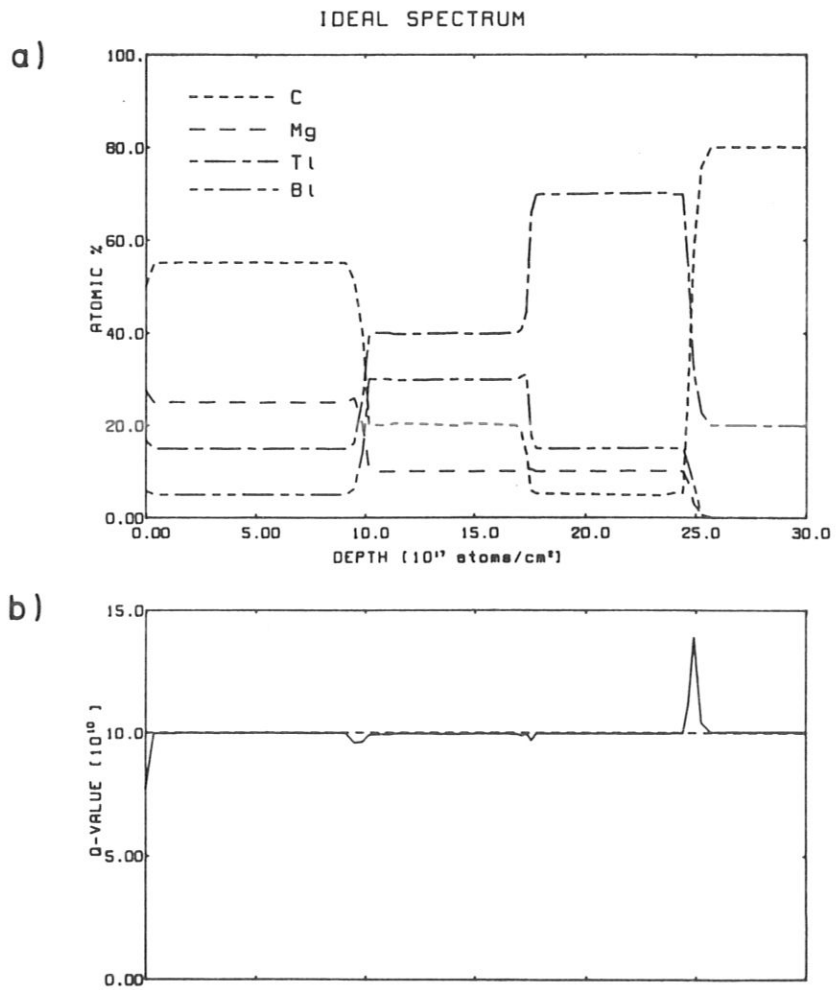


Fig. 14: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 13. Aarhus-version.

a) Relative concentrations vs. depth of C (---), Mg(— — —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

b) When the various isotopes of the target elements are included, even the ideal spectrum (particularly at surface/interfaces) is perturbed because of the isotopic mass differences. Figure 15 shows the ideal spectrum calculated assuming the natural isotopic ratios, and SQUEAKIE yields a targetcomposition which is correspondingly perturbed (Fig. 16a). As also illustrated by the variation of Q with depth (Fig. 16b), the perturbation is quite small.

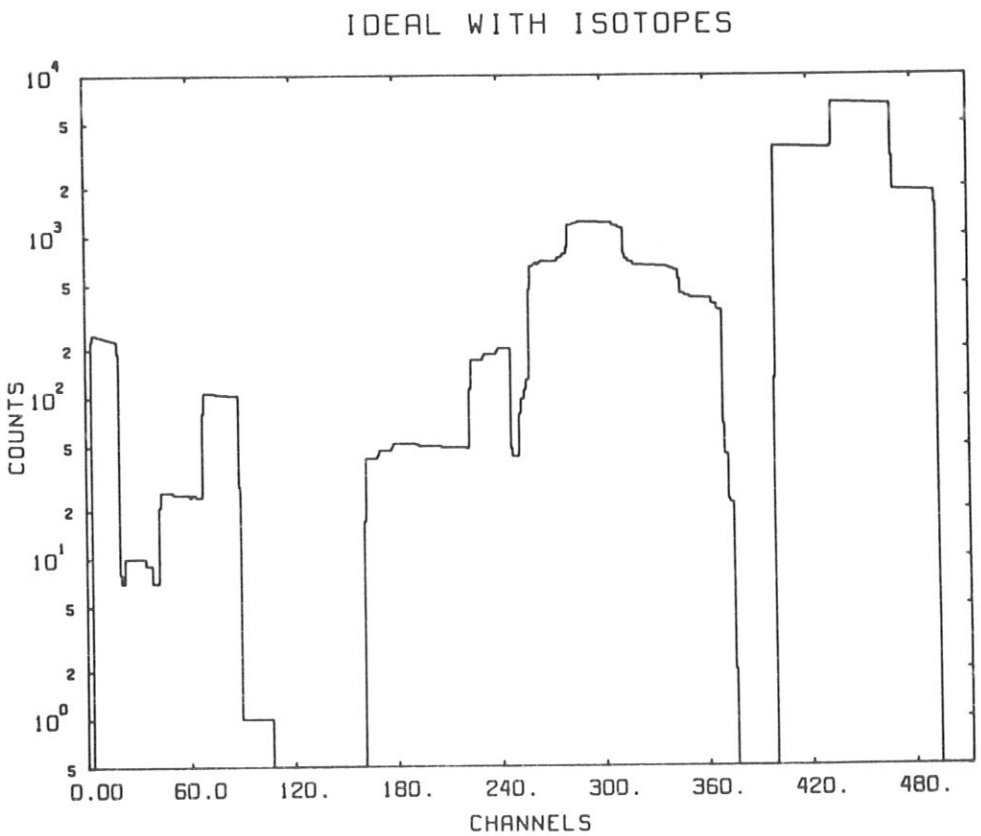


Fig. 15: Synthesized RBS-spectrum, ideal case but including isotopes. Compare Fig. 13.

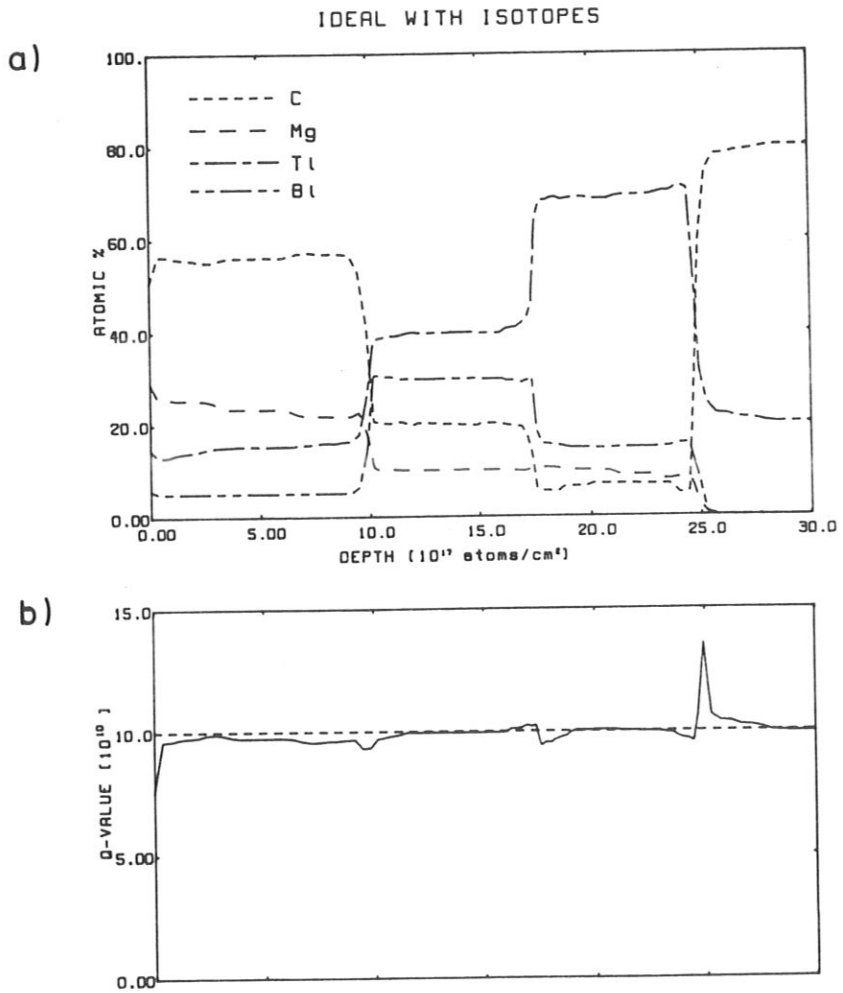


Fig. 16: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 15. Aarhus-version.

a) Relative concentrations vs. depth of C (---), Mg(— —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

c) For RBS analysis of reasonably thin targets with MeV-beams the effect of energy straggling on the ions is usually rather small. As we see in Fig. 17, the resulting smearing of the edges in the spectrum is in our case less than that caused by the isotopic mass differences. Correspondingly also the derived targetcomposition remains quite accurate (Fig. 18a).

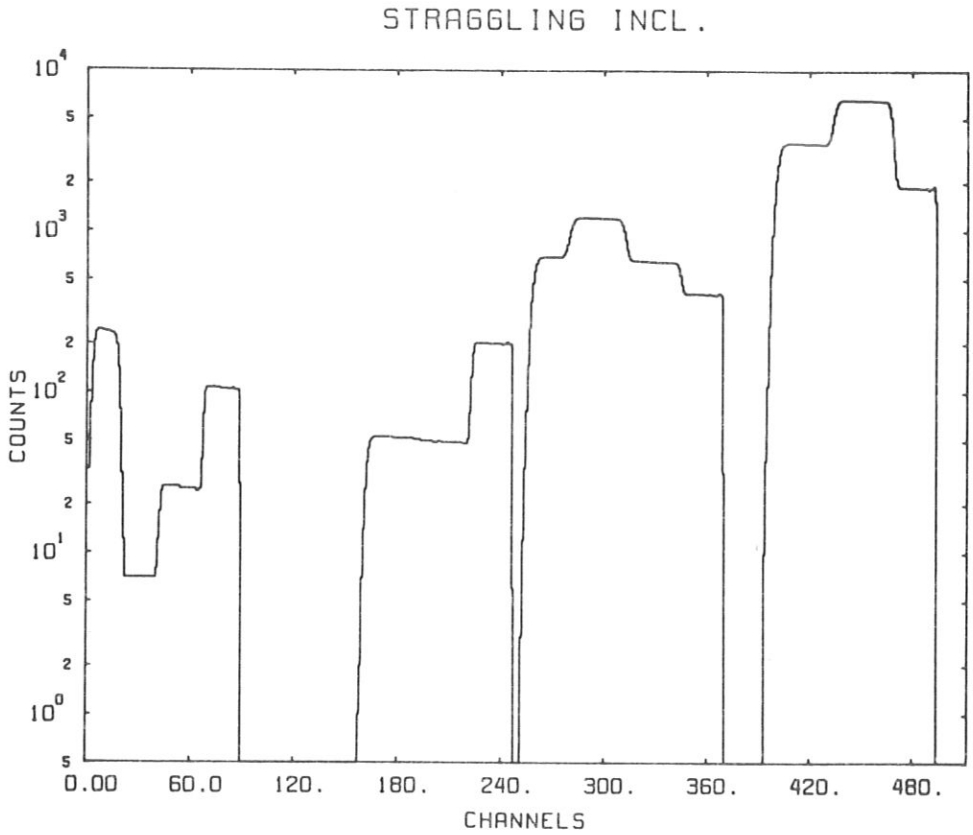


Fig. 17: Synthesized RBS-spectrum, including energy loss straggling. Compare Fig. 13.

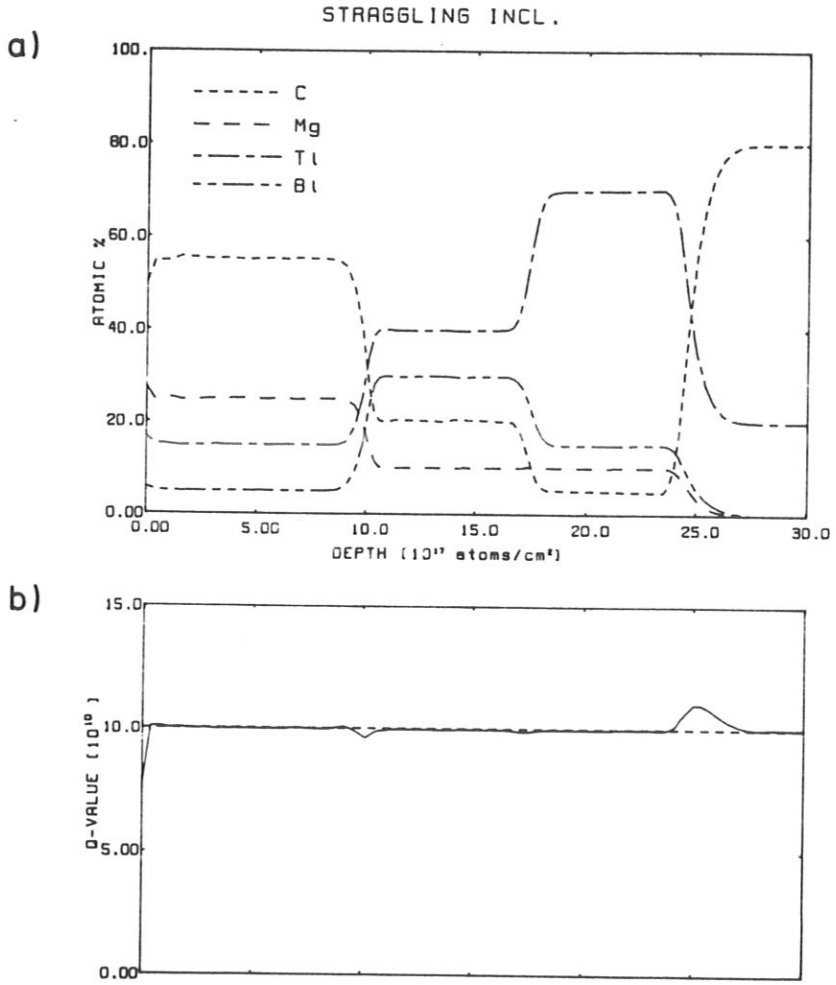


Fig. 18: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 17. Aarhus-version.

a) Relative concentrations vs. depth of C (---), Mg (— —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

d) If we include an energy resolution of ∿ 16 keV of the experimental system, the features are of course all somewhat more smeared (Fig. 19), and so is the resulting targetcomposition (Fig. 20a). However, even with all the above effects combined (also isotopes), the spectrum (Fig. 21) yields a reasonable description of the true targetcomposition (Fig. 22a).

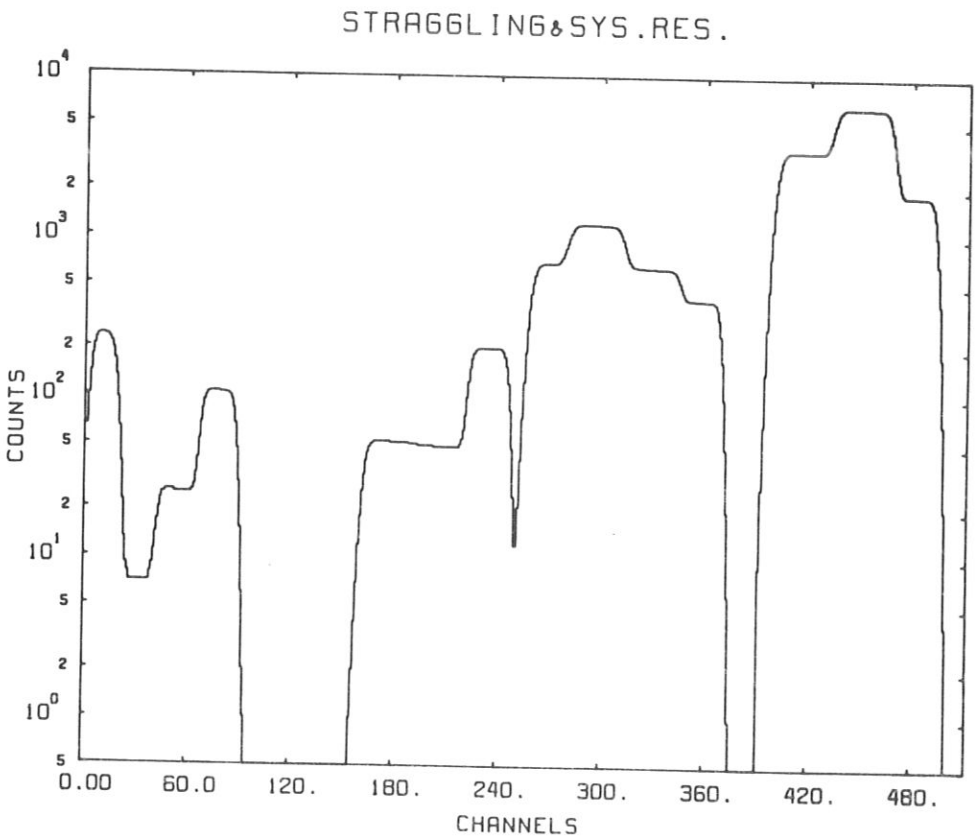


Fig. 19: Synthesized RBS-spectrum, including energy loss straggling and system resolution.

Compare Fig. 17.

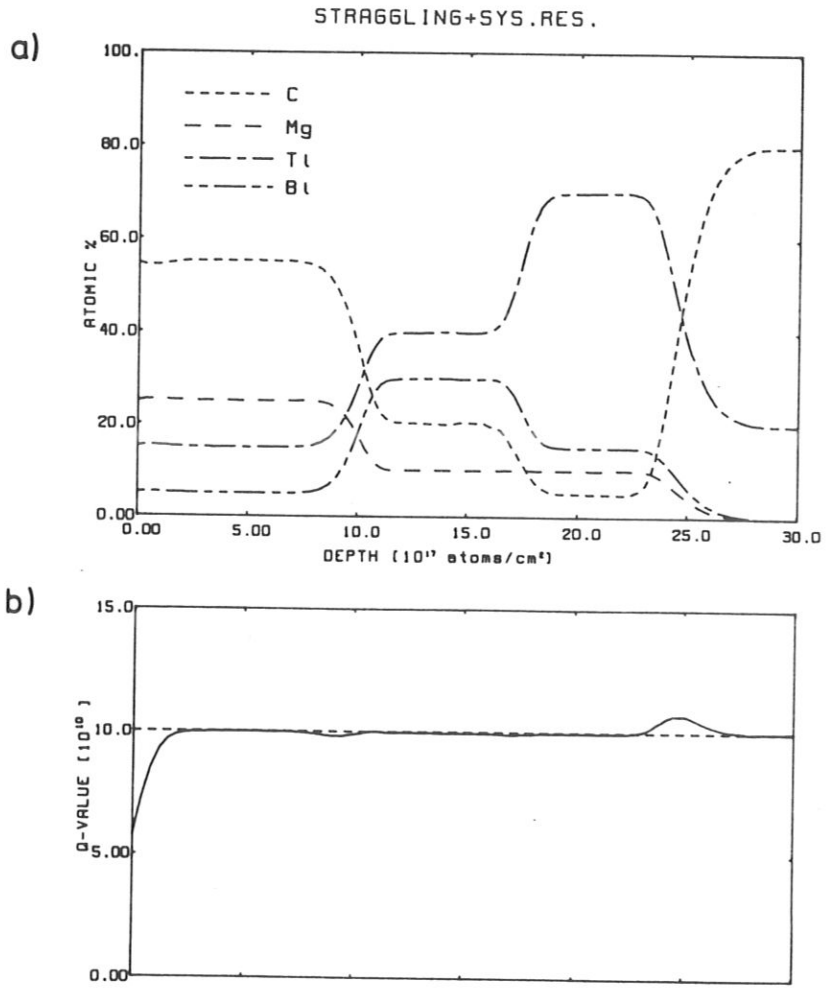


Fig. 20: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 19. Aarhus-version.

a) Relative concentrations vs. depth of C(---), Mg(— —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

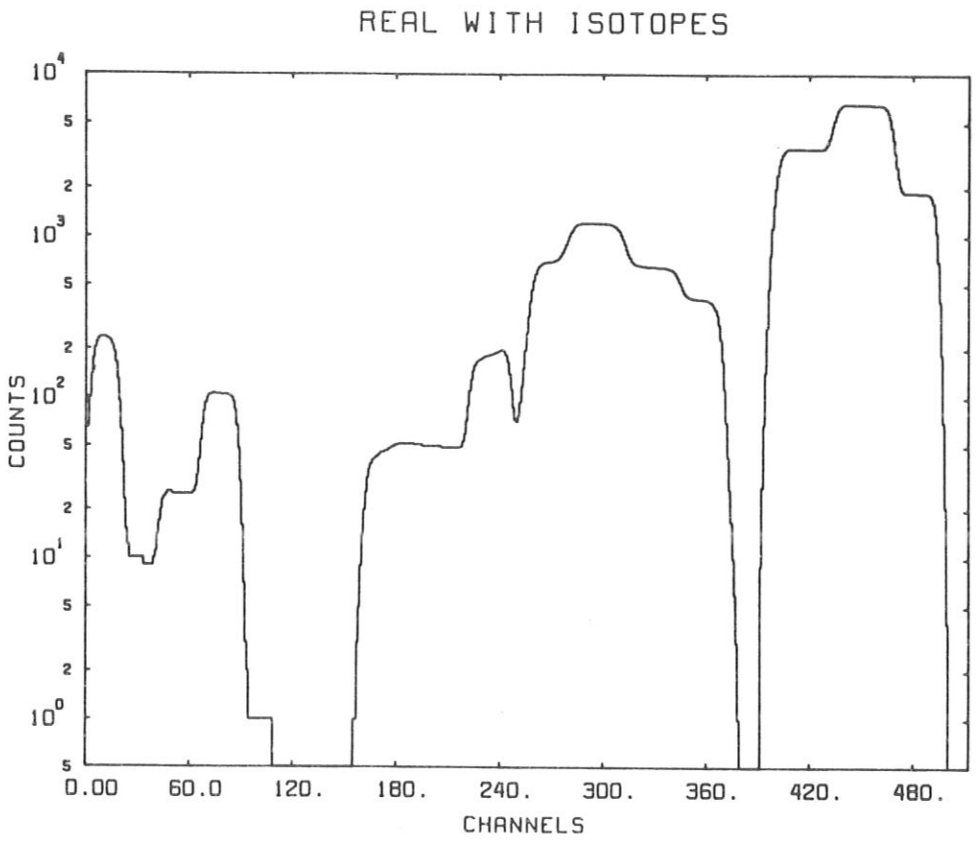


Fig. 21: Synthesized RBS-spectrum, including energy loss straggling, system resolution and isotopes.

Compare Fig. 19.

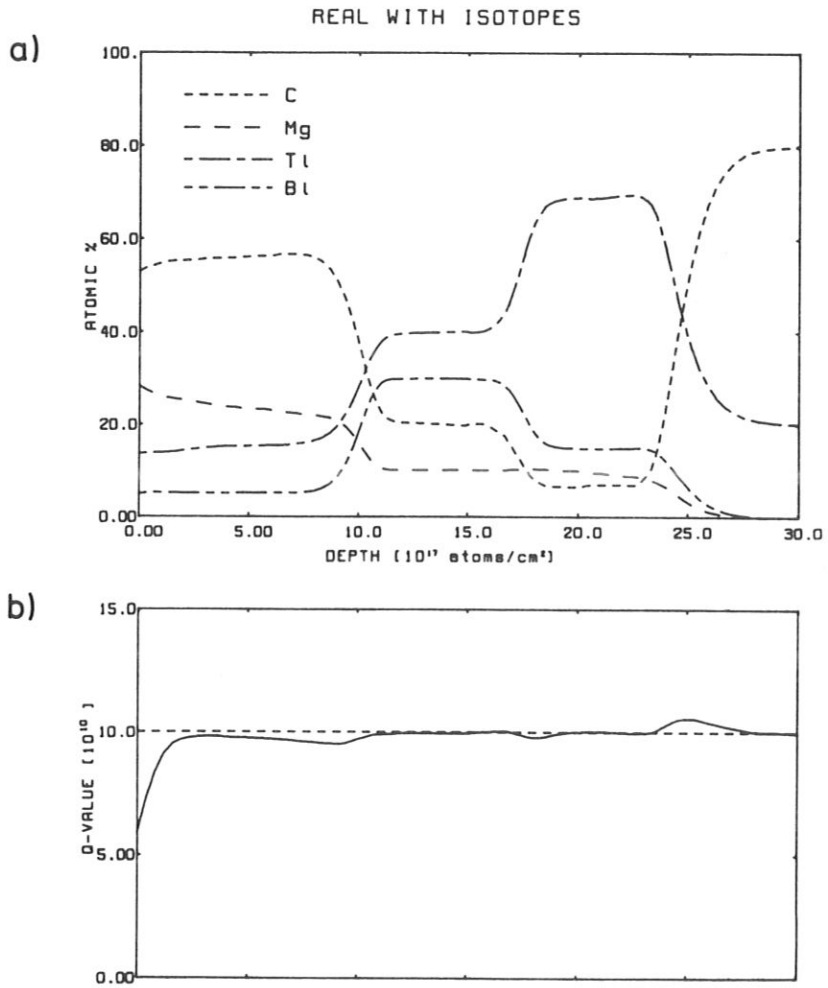


Fig. 22: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 21. Aarhus-version.

a) Relative concentrations vs. depth of C(---), Mg(— —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

e) We may conclude that in this quite representative case, energy loss straggling is of minor importance, system resolution simply causes the expected smearing of depth distributions, whereas isotopic mass differences may also result in perturbations of the stoichiometric coefficients in general.

In a realistic experiment, however, we shall expect the statistical errors in the experimental countrates to be a more serious problem. This question was already discussed somewhat in Ref. 1, but not sufficiently tested. The spectrum of Fig. 21 was therefore calculated again using a particular facility of the computerprogram /8/: In the individual channels the countrate H_i was superposed with a statistical error obtained from a random generator. The spectrum (Fig. 23) therefore exhibits the statistical fluctuations which one would expect to find experimentally.

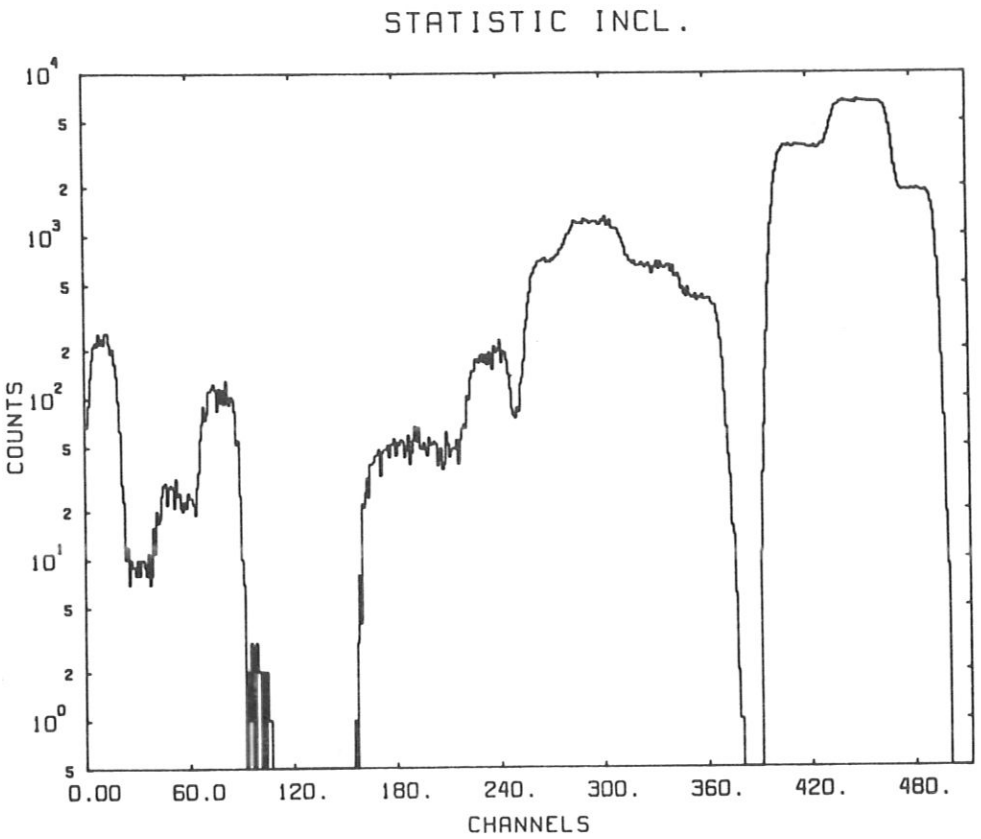


Fig. 23: Synthesized RBS-spectrum, including energy loss straggling, system resolution, isotopes and counting statistics.

Compare Fig. 21.

The resulting targetcomposition (Fig. 24a) of course reflects these fluctuations, but only to the degree expected (Ref. 1); i.e. we may still extract a reasonable estimate of the targetcomposition. Of course, the result may be improved by measuring to larger countrates, if possible.

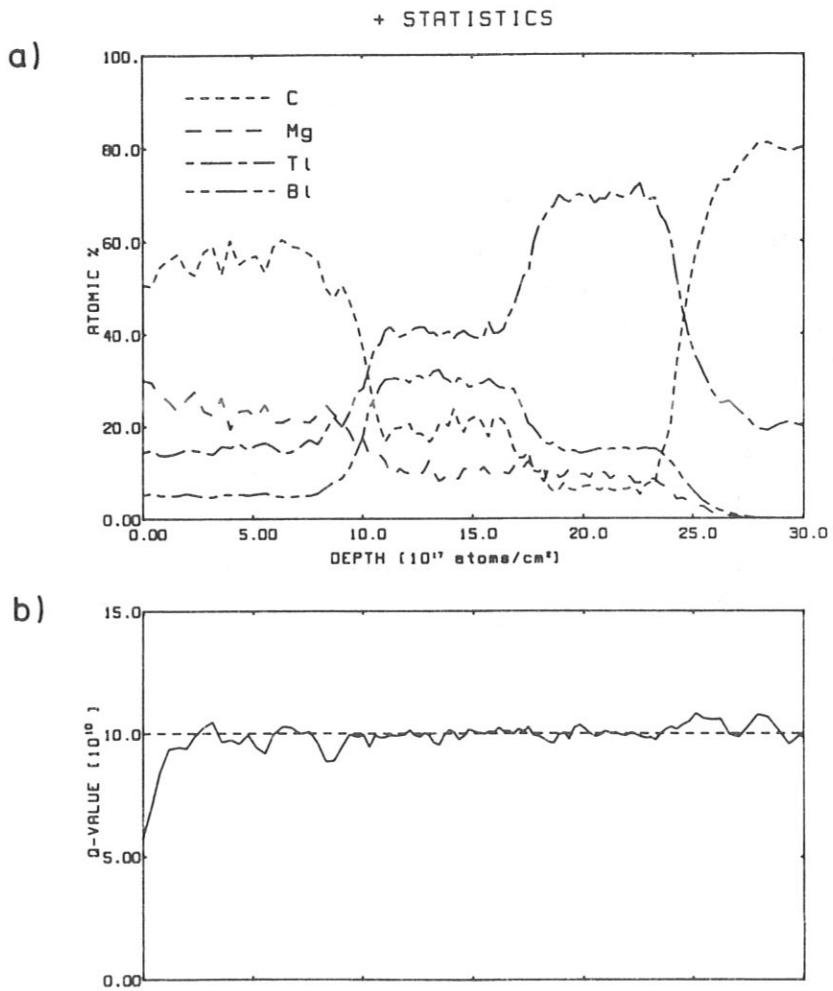


Fig. 24: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 23. Aarhus version.

a) Relative concentrations vs. depth of C(---), Mg (— —), Ti (- — - —) and Bi (-- — --).

b) Eigenvalue Q vs. depth.

iii. The main purpose of the program is the evaluation of depth-distributions, and as discussed in Ref. 1 this is limited towards very thin films by the total experimental resolution. The program does have a facility for deriving the total contents of elements concentrated within the depth resolution (see Sect. 3.3), but if such contents are the only ones in question much simpler programs are available.

The evaluation of thin-film spectra was tested with synthesized RBS-spectra from a target consisting of a $Al_{0.7}$ $Co_{0.2}$ $Au_{0.1}$-film on a C-substrate. Spectra were calculated for the filmthicknesses 10^{18}, $2 \cdot 10^{17}$ and $1 \cdot 10^{17}$ atoms/cm^2 (Figs. 25-27), assuming the same resolution-effects and experimental parameters as above.

As expected, the thickest film allows a good evaluation of the targetcomposition (Fig. 28), but also a rather thin film leads to a reasonable estimate of the surface-stoichiometry (Fig. 29). The latter result benefits from a partial 'cancellation of errors' /1/, which is possible until the film is so thin that the substrate-signal (due to resolution-broadening) seems to indicate larger amounts of C on the surface (Fig. 30). However, even for the $1 \cdot 10^{17}$ atoms/cm^2-film the ratio $n_{Al}:n_{Co}:n_{Au}$ between the concentrations (ignoring n_C) remains essentially correct also in depth. The depthscale, of course, is strongly perturbed by the resolution.

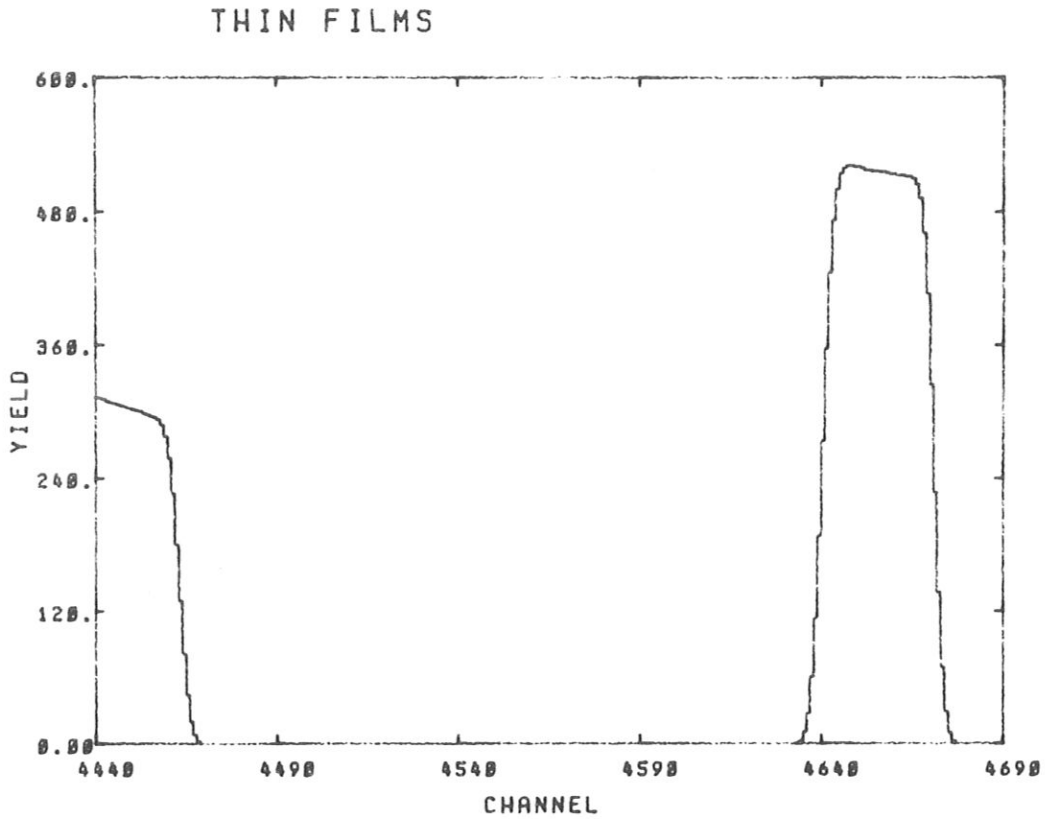


Fig. 25: Synthesized RBS-spectrum for 2 MeV $^4He^+$-ions incident on 10^{18} atoms/cm^2 of $Al_{0.7}$ $Co_{0.2}$ $Au_{0.1}$ on a carbon-substrate. $N_{prim}\Delta\Omega = 10^{11}$, $\theta = 161^\circ$, $\alpha = 19^\circ$, $\beta = 0^\circ$, ΔE_1 = 3.3 keV/channel and 230 keV in channel Ø.

Energy resolution ∿ 16 keV.

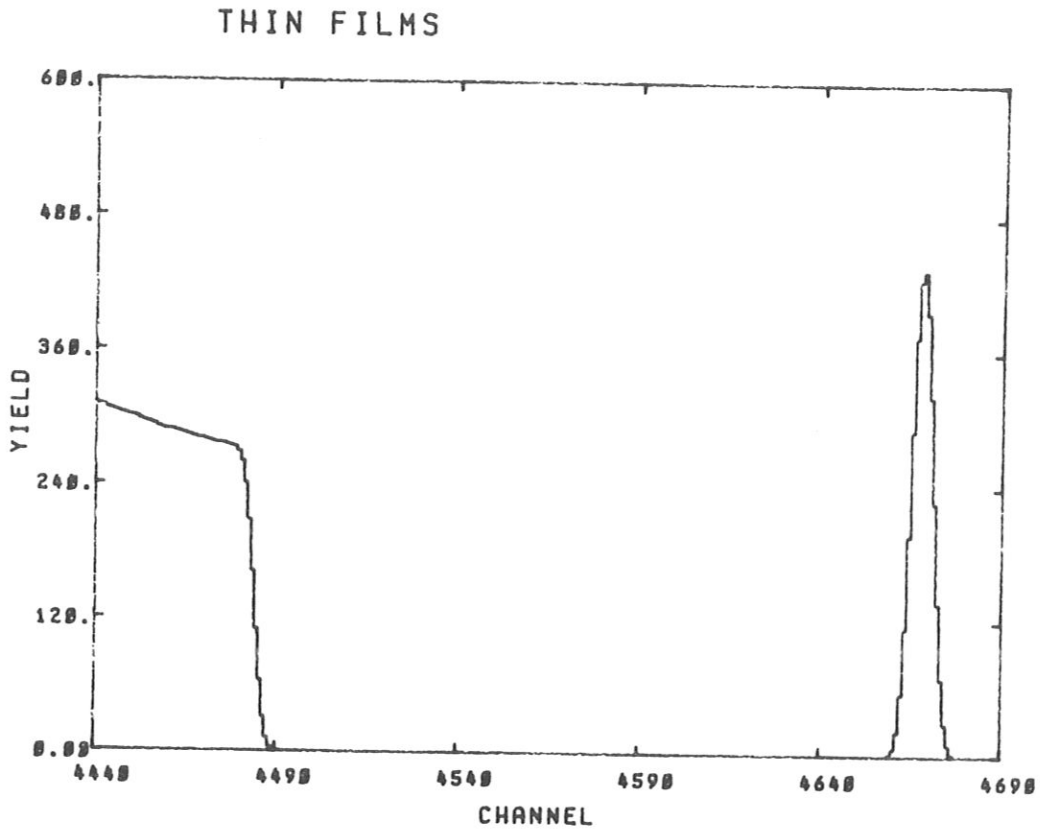


Fig. 26: As Fig. 25, but filmthickness now $2 \cdot 10^{17}$ atoms/cm^2

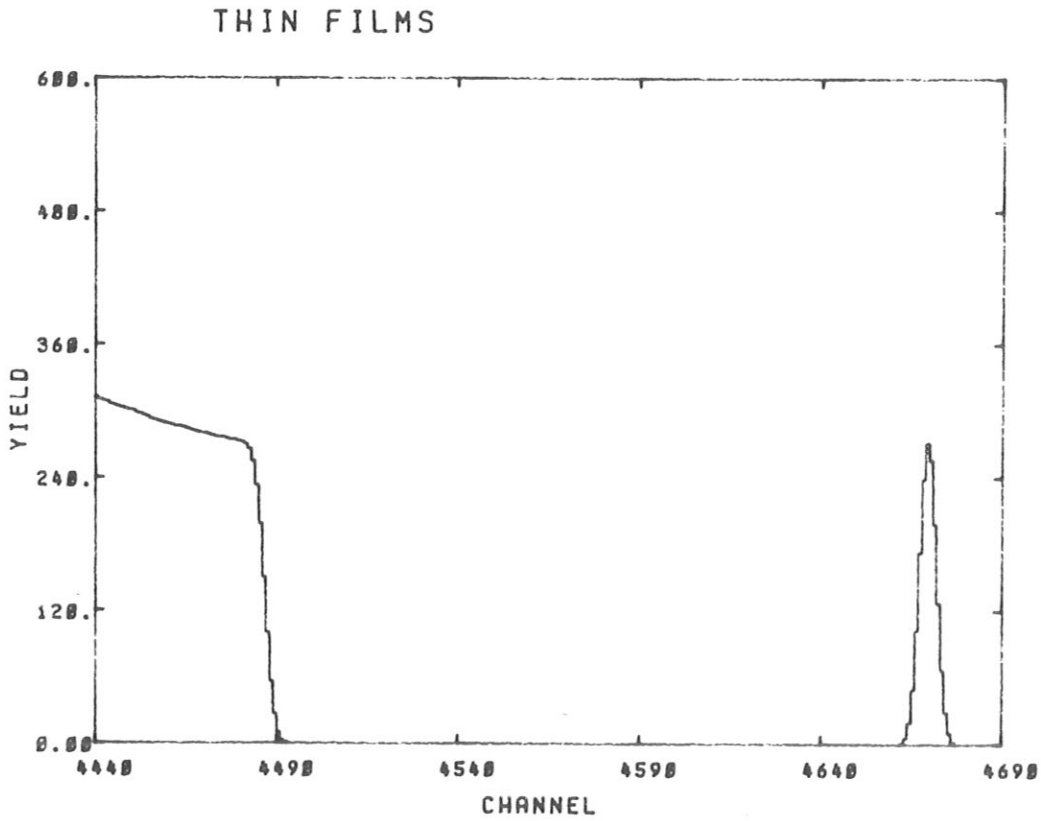


Fig. 27: As Fig. 25, but filmthickness now $1 \cdot 10^{17}$ atoms/cm^2.

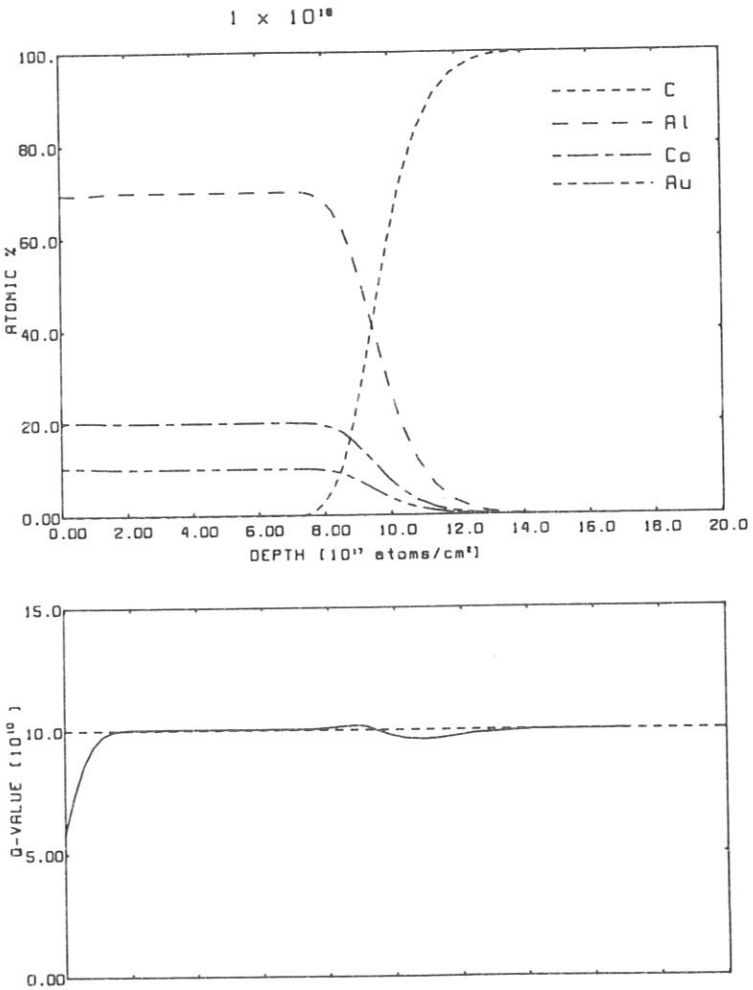


Fig. 28: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 25.

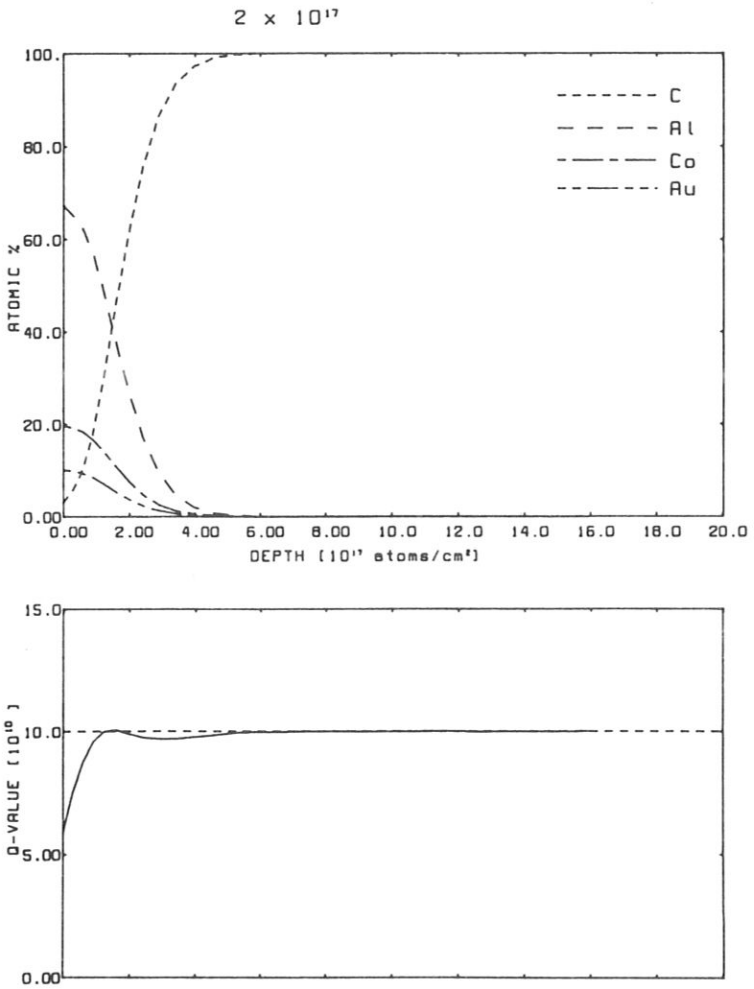


Fig. 29: Plot of SQUEAKIE-output resulting from evaluation of spectrum in Fig. 26

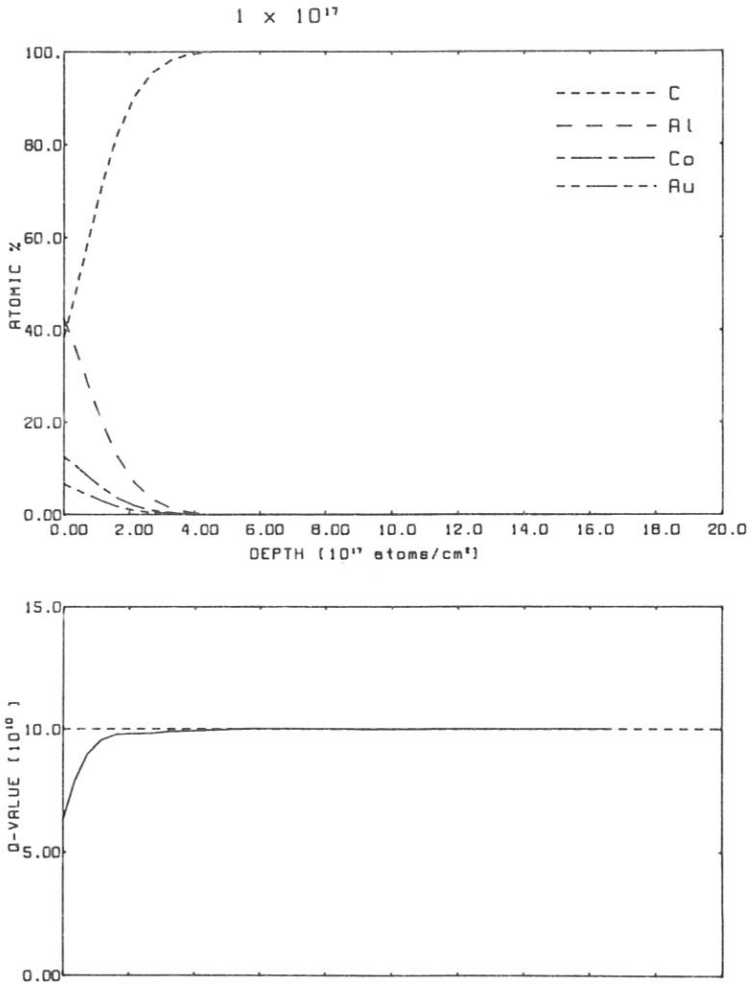


Fig. 30: Plot of SQUEAKIE output resulting from evaluation of spectrum in Fig. 27.

For all three filmthicknesses the total amounts of each element in the film (and thus the filmthickness) are estimated from the total scattering yields (Sect. 3.3) to within $\sim$ 5 %. In contrast, of course, the summation of stoichiometric coefficients (Eq. 3.1) works best for the thick film: For the $1 \cdot 10^{18}$ atoms/cm^2 the total amounts are correct within less than 1 %, whereas for $2 \cdot 10^{17}$ atoms/cm^2 the errors increase to $\sim$ 15 %, and for $1 \cdot 10^{17}$ atoms/cm^2 the total amounts are underestimated by 30 - 35 %.

8. RESUMÉ

The present computerprogram is capable of evaluating RBS-spectra in which the individual signals from the targetcomponents may be distinguished. A spectrum, in which each signal is clearly separated from the others (Fig. 31a), may therefore be directly evaluated without previous analysis. If, however, a signal is superposed on another (Fig. 31b), some kind of separation or background subtraction is necessary. The Aarhus-version of the program has facilities for a simple background subtraction, whereas in Garching this must be performed by a separate program. In any case such problems require a certain insight from the user, and are often too complicated for a simple treatment (Fig. 31c).

The program is primarily intended for the purpose of extracting the depth distributions of the targetelements. For rapidly varying targetcompositions the results will of course be smeared by resolution effects, and for very thin targets the total amounts may be evaluated by means of much simpler programs.

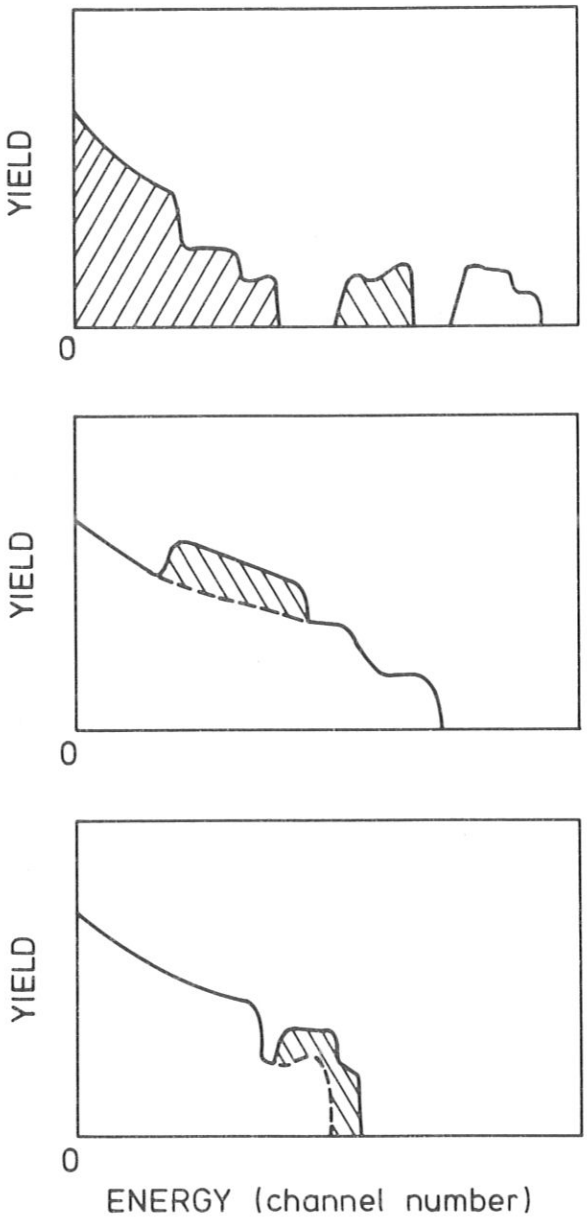


Fig. 31: Examples of RBS-spectra, principle.

a) Directly applicable as input: Separate signals from each element (here 3).

b) Applicable after simple backgroundsubtraction: Signals from two different elements overlap.

c) Only applicable after previous (advanced) analysis: Overlapping signals of varying structure.

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