A SIMPLE METHOD FOR CALCULATING THE NUMBER OF ATOMS IN ION IMPLANTED SAMPLES FROM THE RBS YIELD

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Abstract- A simple method that computes the number of atoms in implanted samples from the integral of the elastic backscattering yield, using a pocket calculator, is represented. The energy dependence E^{-2}, of the Rutherford law and the screening of the nuclear charge by the electron cloud is considered. The method is based on the assumption that the stopping power is a linearly decreasing function of the energy in the range from 1.4 MeV to 2MeV. The total yield can be integrated analytically, and the number of atoms in the sample can then be ascertained by an iteration procedure that can be accomplished with a scientific pocket calculator. The results obtained are compared with the values obtained using the computer simulation code for RBS spectra RUMP.

Keywords-- RBS, Elastic backscattering, Stopping Power

1. INTRODUCTION

Rutherford backscattering spectrometry (RBS) is a commonly used technique for analyzing the near-surface region of solids. The technique is well understood and provides a quick and accurate analysis in described the technique [1-3] in detail, although the problems associated with using RBS on insulating materials are not discussed adequately. When fast protons are backscattered from a sample, one can deduce the number of atoms per unit area, Na_f, from the integral (or peak area) of the signal in the backscattering spectrum

$$Na_f = \frac{Y_{tot}}{n\Omega\sigma(E_0)}\cos\alpha \qquad (1)$$

Y_{tot} is the total RBS signal, α the angle between the incident beam and the normal to the target surface, n the total number of incidenting ions, Ω the solid angle of detection, and $\sigma(E_0)$ the Rutherford scattering cross-section which depends on the energy E_0 before scattering. N is the atomic density of the sample, which is not precisely known and a_f is sample thickness; and Hence N a_f, is the number of atoms per unit area in the sample. N a_f is usually expressed in atoms per unit area. Therefore, the sample thickness is directly obtained in length units in an RBS experiment once a value for the atomic density is assumed. σ is dependent on E_0 but it also depends on the incident particle and target atom mass M_1, M_2 and atomic number Z_1, Z_2 respectively, and the collision angle, θ.

A factor that can make (1) inaccurate is the screening of the electrostatic potential of the target nucleus by its atomic electrons. This effect can important even if the distance of closest approach between projectile and target nuclei is smaller than the K-shell radius [4], which is normally the case in a typical RBS experiments. Approximation methods taking into account the electron shells are used to deal with the scattering by a screened

potential. The screened scattering cross section $\sigma_s(E)$ is generally compared Rutherford's value, $\sigma(E)$, by a screening factor s through the relation :

$$\sigma_s(E) = s\sigma(E) \tag{2}$$

Most of the reports include analytical calculations based on the application of Rutherford's formula to thin slices of material into which the sample is conceptually split. It is assumed that the energy stopping cross section is constant in each slice, and its dependence on energy is obtained from polynomial fits of the stopping power of either existing or interpolated data, according to empirical scaling laws [5]. A simulation code for RBS spectra is quite convenient for quantitative RBS analysis, as it may reveal details that, otherwise, could be overlooked if the analysis is done by hand. Therefore it is extremely important to be aware of the limitations and sources of error the computer analysis might have [5].

In this work a simple method, using pocket calculator, is put forward for the determination of the amount of atoms in ion implanted samples. The purpose of this method is not meant to do the job that any of existing computer codes does. Its goal is to produce a precise value of the thickness of a layer without the need of simulating a spectrum, once the integral of its RBS signal is ascertained. In this method, the calculation takes into account the E^{-2} energy-dependence of $\sigma(E)$ and the electronic screening of the target nucleus. The latter correction is not taken into account in most of the existing computer codes. An analyzing $^4He^+$ beam an energy of 1.89 MeV is used, and the backscattered particles are detected by an ORTEC silicon barrier detector, mounted at a scattering angle of 150°.

2. CHOICE OF THE SCREENING FACTOR

Depending on the approximation used to obtain the screened cross section, different expressions for s can be procured. In the derivation of the screened scattering cross section two main approximations are usually applied, which depend on the projectile velocity, v. If v is much greater than $Z_1 v_k$, where $v_k = Z_2 v_0$, v_0 being Bohr's velocity, the first Born approximation is used [8]. On the other hand, if v is much smaller than $Z_1 v_k$, a classical description of the scattering process can be used [8]. It is interesting to note that for 2 MeV α particles; a standard particle and energy in a typical RBS experiment, v is approximately equal to $Z_1 v_k$, when the target atoms are Li. Therefore it would seem that for low Z_2 both approximations is in felicitous; nevertheless, as both approximations converge to Rutherford's value for high values of v, the classical approximation is generally used [9]. Most of the approximations used for the derivation of the screened cross section in the energy range from about 0.2 MeV up to 2.2 MeV are discussed by Andersen et al. [10]. Their experimental results are in good agreement with exact classical differential-scattering cross sections based on the Lenz-Jensen and Dirac-Harree-Fock-Slater (DHFS) atomic potential [11]. They also compare these values of screening with simple analytical expressions for backscattering of He from a heavy atom such as Bi. The results obtained from their work allow one to use one of the simple analytical expressions for the screening factor in the energy range of interest in RBS, with the confidence of having values for the screening with errors of the order of 0.5% for the worst case. The screening factor used in the present work [10] is

$$s = \frac{1}{1 + \dfrac{V_1}{E_{CM}}} \tag{3}$$

where E_{CM} is the total kinetic energy in the center-of-mass reference frame and

$$V_1 = 48.73eVZ_1Z_2\left(Z_1^{2/3} + Z_2^{2/3}\right)^{1/2} \tag{4}$$

The straightforward expression, obtained using the Lenz-Jensen screening function, is scattering angle independent and is more accurate for backscattering angle; close to π.

The screening factor can be expressed as a function of the projectile's incident energy in the laboratory reference frame (E). Therefore, by analogy with (3), are write

$$s = \frac{1}{1 + V_0/E} \tag{5}$$

where V_0 is $[(M_1 + M_2)/M_2] \, V_1$,
This correction is usually lower than 0.05% and is therefore negligible.

Supposing that the atomic density, N , is constant across the sample, in general the total yield, Y_{tot} , will be

$$Y_{tot} = n\Omega \int_0^{Na_f'} \sigma * (E)d(Na') \tag{6}$$

where Na'_f is the total inwards path length of the projectile inside the sample of thickness N a_f, i.e. $a'_f = a_f/\cos$, and d(Na') defines a shallow region in the sample of thickness d(Na), thin enough for E to be considered to be constant in this region. From the definition of the stopping power, $\varepsilon(E) = -dE/d(Na')$. it is possible to rewrite (6) as

$$Y_{tot} = n\Omega \int_{E_0}^{E_1} \sigma * (E)d(-dE/\varepsilon(E)). \tag{7}$$

Note that the integral limits E_0 and E_1 are the projectile energies before the collision at the surface of the sample and at the depth N a_f, where the inner interface of the sample is located (path length N a'_f), respectively. This integral can be solved analytically if a convenient form for the dependence of the stopping power on energy can be obtained.

3. LINEAR STOPPING POWER APPROXIMATION

As can be seen from the schematic representation in Fig.1, the stopping power function for He has a characteristic energy dependence for the most of the elements with a broad maximum somewhere near 1 MeV [1,2]. In the energy range of interest, (1.4 to 2 MeV), this function is very well described by a straight line of negative slope, given by
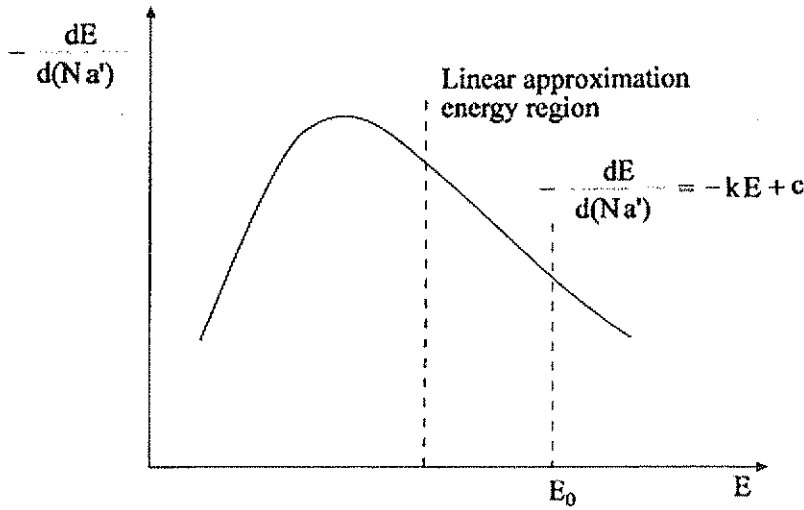
$$-dE/d(Na') = -kE + c. \tag{8}$$

Figure 1. A schematic of how the stopping power depends on projectile energy. Broken lines depict the energy region where the linear stopping power approximation is used.

As a result of this one has a simple relation between the amount of material traversed by the projectile and the energy it loses, given by

$$d(N a') = \frac{dE}{k E - c} \qquad (9)$$

This equation with the condition that for N a' = 0 we must have E = E_0, gives the relation between path length and energy of the projectile. For the path length N a'$_f$ it is

$$N a'_f = \int_{E_0}^{E_1} \frac{dE}{kE - c} = \frac{1}{k} \ln \frac{c - kE_1}{c - kE_0} \qquad (10)$$

In addition, (9) allows the integration in (7), and if we write the screened cross section as

$$\sigma * (E) = \sigma(E_0) E_0^2 \frac{1}{E^2 + V_0 E} \qquad (11)$$

the integral can be solved analytically, giving:

$$Y_{tot} = n\Omega\sigma(E_0) E_0^2 \left[\frac{1}{V_0 c} \ln\left(\frac{E_0}{E_1}\right) + \frac{k}{c(c + kV_0)} \ln\left(\frac{k E_1 - c}{k E_2 - c}\right) - \frac{1}{V_0(aV_0 + c)} \ln\left(\frac{E_0 + V_0}{E_1 + V_0}\right) \right] \qquad (12)$$

From (12) it is possible to obtain E_1 once Y_{tot} is known, and from (10) one obtains N a'$_f$ and N a$_f$.

The linear approximation of the stopping power beyond its maximum has been used in some cases to obtain the thickness of a sample from the spread in the energy of its RBS signal [12]. This approach has the advantage that there is no need to know the irradiation dose or the detector's solid angle to perform the calculation. It has, however, the following disadvantages: the inwards and outwards trajectories of the projectile in the sample are involved, and on the way out the energy will correspond to stopping

powers near the maximum, and a second linear approximation may be necessary. This will especially be the case for light elements with a low kinematic factor. This fact also limits the maximum thickness of the implanted sample for which the approximation is good. In general this procedure is more sensitive to stopping power inaccuracies, as the energy lost by the projectile is evaluated on the way in and on the way out of the sample. Moreover, the calculation can be performed only when the gain of the amplifiers has been calibrated in number; of keV per channel. This parameter (i.e. keV/channel) is most conveniently measured by taking a spectrum of a light substrate, thinly coated with heavier elements (preferably monoisotopic), which will be well spaced over the whole spectrum. A reference sample has been made of polished graphite coated Al, Cu and Au. By plotting the kinematic factors for each element against the channel number at which they occur (half-height edge for C, peak for O, Al and Cu), a linear least squares fit can be used to draw a line through the data points. The gradient of the line (when multiplied by the beam energy) gives the keV/channel.

If the thickness of the sample is computed from the total yield according (12), the scattering experiment has to be very well calibrated, including dose and detector solid angle. In principle, using the reference sample, it is "possible to measure these parameters with an uncertainty of better than 2% [6-7]. In this case there is no need for the energy calibration of the detection system to evaluate the thickness of the sample. As only the inwards trajectory of the projectile is involved, the linear approximation will still be good for much thicker samples than in the previous case, and will be less affected by the lack of a precise knowledge of the stopping power.

The determination of the thickness of a sample from its RBS yield, according to the approximations aforementioned, relies, thus, an solving (12) for E_1. As this equation is transcendent it has to be solved numerically. Some scientific programmable pocket calculators (i.e. Casio fx-4500p) have a root finder built-in application that can be solving for any variable in an equation, and therefore can be used to make such determinations.

Although this method can determine N a_f with great precision, there is the problem of the accuracy as in any measurement. Besides the calibration problems mentioned previously: current integration and detector's solid angle, the uncertainty in the values of the stopping power for He^+ remain ±5-10% according [6-7] It should be emphasized that there are discrepancies in the tabulated values for this stopping power comparing [1] with [3]. The stopping power will change as more ε_r is implanted and this requires iteration of the yield equation. A new fit to $d\varepsilon/dx$ is required each time..

4. RESULTS

After careful calibration of the energy scale of the spectra and normalisation to the incident number of projectiles total yields are calculated from the RBS measurements using surface energy approximation. As might be expected it is impossible to show spectra of each sample here. Therefore we will give a spectrum as an example as this is typical of the spectra of each target material (see fig. 2). The number of atoms per cm^2 is determined using (10) and (12) for several total yields. The values acquired are compared with results given by a computer code simulating RBS spectra not taking into account the screening effect. The purpose of the comparison is twofold; first, when the screening is small, as for light or medium elements, it will serve

as a check of the maximum thickness for thick the linear approximation is valid. On the other hand, when the screening is important, as in heavy elements, it will -exhibit- how important this correction is. For this purpose, the simulating RBS spectra, programme RUMP [13] version 3.5 was used.   This RUMP code, modified to work in a microcomputer environment, is commercially available. This program has incorporated a fifth order polynomial fit of empirical stopping power values [14].
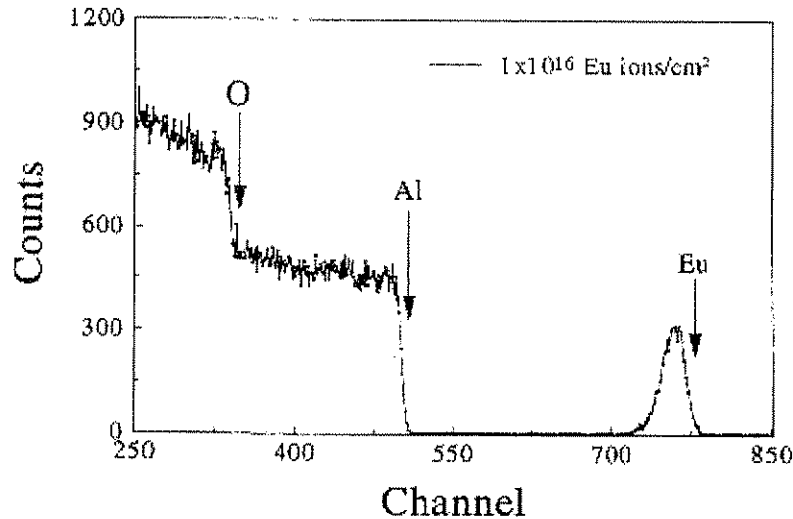

Figure 2. 1.89 MeV 4He+ backscattering spectra from sapphire implanted sample. The calculated RBS edge positions are shown for the main elements.

Table 1 shows the thickness of an Eu implanted Al_2O_3 sample for a given total yield. The stopping power values used in this table are those from [3], giving k=1.9243x10^{-5} (10^{-14} cm^2) and c=183.34 (10^{-14} eVcm^2). The total yield is obtained for Ω = 0.42msr, integrated current 50 μC, α=0°, and stated previously, E_0=1.89 MeV and θ=150°. Comparing the thickness values in the third and the fourth columns, it can be seen that when the screening correction is considered, a given total yield gives rise to a thicker sample an expected. Thus the correction becomes less important for thicker samples. As can be seen from the Table 1, there is a difference in thickness of 2.94% and 1.37% for yields of 8x10^1 and 8x10^4, respectively. This result is a consequence of the stronger dependence on E of σ than of s. As it is known, there is a discrepancy of about 10% in the stopping power values according to different authors. In order to test the effect that this uncertainty in the stopping power may have in the evaluation of the thickness of a sample, the same calculations have been done when the linear stopping power approximation is obtained from the tabulated data in [1], Table 2 shows the results obtained using these data. The straight line are now k=1.5820x10^{-5} (10^{-14} cm^2) and c=158.23 (10^{-15}cm^2). Comparing the data in Tables 1 and 2, it can be seen that in spite of the discrepancy in the stopping power values, the difference in the calculated thickness of the sample from the total yield is very small.

Table 1.   Thickness of Eu implanted Al_2O_3 samples obtained from a given total RBS yield. Stopping power values are taken from [1].

Y_{tot}*	$N\,a_f$ / 10^{15} at.cm^2			E_1/eV**
	Surface Energy Approximation	Energy Correction without Screening	Screening Correction	
8×10^1	1.071	0.99	1.00	1905163
8×10^2	10.71	11.90	12.20	1856615
4×10^3	53.60	49.80	50.80	1758940
8×10^3	112.12	99.20	100.20	1639552
8×10^4	1073	1020.40	1030.27	1299993

* Y_{tot} = total number of counts
** E_1/eV = The energy before collision at the inner interface

Table 2.   Same as Table 1, but using the stopping power values from [3]

Y_{tot}*	$N\,a_f$ / 10^{15} at.cm^2			E_1/eV**
	Surface Energy Approximation	Energy Correction without Screening	Screening Correction	
8×10^1	1.071	0.99	1.01	1755194
8×10^2	10.71	11.95	12.21	1707741
4×10^3	53.60	51.25	52.45	1640927
8×10^3	112.12	100.02	100.20	1630312
8×10^4	1073	1045.27	1050.35	1240427

Table 3 depicts the total yield generated by RUMP for the Eu implanted samples having the thickness as in the third and fourth columns in Tables 1 and 2. As can be seen, there is a good agreement between the total yield from the which thickness of the Eu implanted sample is obtained, using the linear approximation without screening (i.e. the third column in the Table 1) and the total yield generated by RUMP for the corresponding thickness. On the other hand, when the screening is introduced, there is systematic discrepancy in both values, giving RUMP higher total yields, as expected, due to the fact that the simulation programme does not include the screening effect.

Table 3.   Total yield generated by RUMP for Eu implanted Al_2O_3 samples having thicknesses as shown in Tables 1-2.

Eu N a_f 10^{15} at./cm^2	RUMP Y_{tot}	Eu N a_f* 10^{15} at./cm^2	RUMP Y_{tot}
0.99	80	0.98	80
1.00	81	0.99	81
11.90	800	11.95	800
12.30	802	12.15	803
49.80	4021	51.72	4027
51.25	4029	52.60	4030
99.20	8015	107.32	8021
101.72	8022	108.42	8027
1020.40	78862	1030.20	78875
1032.25	78878	1047.35	78882

• Stopping power from Tesmer et al. [1]

Finally, it is worth noting from the results in the aforementioned tables that for samples of thicknesses up to about 100×10^{15} atoms/cm^2, the crude surface energy approximation provides more accurate results than just correcting for the E^{-2} dependence of σ, and than can be used with an error lower than 4% for Eu implanted samples of thicknesses up to about 100×10^{15} atoms/cm^2.

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