Calculation for optimization of the experimental conditions for RBS analysis at the HUS 5SDH-2 tandem accelerator

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Abstract. The dependences of the depth and mass resolutions of analysis using Rutherford Backscattering Spectrometry (RBS) on some experimental conditions (such as the beam energy, the target tilting angle, etc.) have been investigated. A computer program for simulating the RBS spectra and for calculating the depth and mass resolution under different experimental conditions was developed. The results of calculation were experimentally checked by using some reference samples. The good agreements between calculated and experimental values have been found. The optimum analysis conditions over a wide range of RBS applications based on our calculation can be chosen. This investigation was conducted by using the RBS system at HUS 5SDH-2 Tandem accelerator at the Hanoi University of Science.

1. Introduction
The HUS-5SDH-2 Tandem Pelletron accelerator system at Hanoi University of Science has been installed and started operating since 2012. It is mainly used for material characterization including RBS, which is very useful for probing the depth profile of near-surface regions of materials.

The purposes of this paper are: (i) to estimate the influence of experimental condition to some parameters by theoretical considerations, (ii) to measure the depth resolutions at various condition and compare them with the calculated values, (iii) to establish the optimum experimental condition. A computer program for calculation has been developed and used for estimation of several parameters such as the energy resolution, the accessible depth and the depth resolution that are under influence of experimental conditions.

All of experiments were carried out using RBS the Tandem 5SDH-2 Accelerator at Hanoi University of Science. In our experiment, RBS spectra collected with the thin gold films on glass substrate have been obtained with various experimental conditions such as energy of the beam and tilting angle of the samples. The calculations have been performed using our computer program at the same experimental conditions and the obtained results were compared with the experimental ones.

2. Theoretical calculations and the RBS simulation code

2.1. The mass resolution
The mass resolution $\delta M_2$ at mass $M_2$ is defined as the ability of the system which can distinguish a minimum value of mass difference. It is related to the separation of energy $\delta E$ between signals in RBS spectra caused by different elements at certain depth as follow

$$\delta M_2 = \frac{\delta E_L}{E_0 \left( \frac{dK}{dM_2} \right)},$$

where $K$ is the kinematic factor and the energy resolution $\delta E_L$ at surface of the sample was obtained from analysis of RBS spectra in the low energy side.

2.2. The accessible depth
The accessible depth in RBS depends on the target compositions, tilting angle, energy of the incoming beam and mass. To satisfy the condition of accessible depth, the backscattered particles must emerge from the target with sufficient detectable energy $E_i$. An arbitrary criterion has been proposed [8]

$$E_i \geq \frac{1}{4} KE_0. \quad (2)$$

Here $E_0$ is the energy of incoming beam.

2.3. The depth resolution
The depth resolution at depth $N_t$ is related to the minimum detectable energy difference $\delta E_H$ of the scattered particles (which is referred as the total energy resolution) and is given by the following formula

$$\delta(N_t) = \delta E_H \left( K e_{in} \frac{1}{\cos \alpha} + e_{out} \frac{1}{\cos \beta} \right), \quad (3)$$

where $K$ is the kinematic factor, $e_{in}$ and $e_{out}$ are the stopping power of the incident and exit beam, $\alpha$ and $\beta$ are the angles between target normal and incident and exit beam, respectively. The total energy resolution $\delta E$ at certain depth is contributed from different sources including the detector energy resolution, energy spread of incoming beam, energy straggling, geometry and multiple scattering effects. Detail expressions for those contributions are given in the appendix.

2.4. The RBS simulation code
A simple simulation computer code named RUT has been developed at our laboratory. The main part of this code is evaluation of energy $E$ of particle having initial energy of $E_0$ after passing through a layer of material. This was calculated by solving the following first order ordinary differential equation by using adaptive step size Runge-Kutta algorithm [11]

$$\frac{dE}{dN_t} = -e(E), \quad (4)$$

with the initial value $E(N_t = 0) = E_0$. The stopping power $e$ can be calculated for a certain energy $E$ using tabulated parameters from the electronic stopping power data by Andersen and Ziegler [2, 3]. The following parameters can be derived from the code: (i) The stopping powers at certain depth, (ii) the kinematic factor (iii) the accessible depth.
3. Experimental arrangement, data extraction

The RBS experiments were performed using the Pelletron Tandem accelerator model 5SDH-2 for thin gold film with thickness of \( 200 \times 10^{15} \text{ cm}^2 \) with the estimated standard error of 10% on glass substrate. The He beam after being accelerated by the Pelletron was focused, collimated and entered the RC43 scattering chamber equipped with a charged particles spectroscopy system. This system comprises a silicon surface barrier detector (energy resolution of 11 keV for 5.486 MeV alpha particle) and the conventional associated electronics. The experimental setup is shown in figure 1. The detector was placed at the distance of 130 mm from the target allowing for a detection solid angle of 3 mSr.

![Figure 1](image)

**Figure 1.** The schematic view of the accelerator and the RBS spectroscopy system equipped in the analytical beam line.

In our investigation only the depth resolution was compared with theoretical calculation. The depth resolution was determined from the spectra obtained with various energies of incident beam for the case of the target tilting angle of 50 degrees and various target tilting angle angles for the case of 2200 keV incident He ions.

The typical RBS spectrum which was used to extract the depth resolution is shown in figure 2. The backscattered signals from the thin Au film were numerically smoothed and their derivations were taken. The obtained spectra were fitted with the Gaussian function for low energy and high energy sides. The fitting interval starting from a point which corresponds 12% of full height and ending at a point which is corresponds 88% of full height was chosen [8]. The depth resolution at the depth \( N_t \) was determined by the following formula [6]

\[
\delta(N_t) = \delta E_L \frac{N_t}{E_H - E_L},
\]

where \( E_L \) and \( E_H \) are the energy resolutions at low energy side and high energy side.
Figure 2. The typical RBS spectra for thin Au film on glass substrate. The high energy and low energy edges from backscattered signals of Au film are indicated.

4. Results and discussion

Figure 3 shows the simulated spectrum obtained by using our code for a sample which consists of some material layers together with a spectrum calculated by the well-known software RUMP [1] for the same sample. It is clearly seen from the figure that two spectra are in good agreement. Beside the simulation of the RBS spectrum, it is possible to use our simulation code to calculate several parameters including the kinematic factor, the accessible depth, the energy loss, the stopping range and the energy resolution at certain depth. From the results of these calculations, one can easily choose an optimal experimental setup in order to get the desired depth, best mass and depth resolutions.

Figure 3. Simulated spectrum of $1.7 \times 10^{18} \text{ cm}^{-2}$ of an Al-Cu alloy on $0.55 \times 10^{18} \text{ cm}^{-2}$ of a Ti-W alloy on a silicon substrate generated by our simulation code (blue line) and RUMP code (red dots).

The theoretical values of the accessible depth calculated by our simulation code were compared with tabulated values taken from Ref. [8]. It is shown in table 1 that they are in good agreement for different beam types and beam energies.
Table 1. Accessible depth for several target material

| Beam | Energy (keV) | Accessible depth (µm) (Calculated by our simulation code) | Accessible depth (µm) (Calculated by Chu [7]) |
|------|--------------|-----------------------------------------------------|---------------------------------|
|      |              | Au | Ag  | Ni  | Al  | Au | Ag | Ni  | Al  |
| $^4$He | 1000        | 0.57 | 0.59 | 0.50 | 0.80 | 0.5 | 0.6 | 0.5 | 1.0 |
|      | 2000        | 1.03 | 1.12 | 0.96 | 1.67 | 1.0 | 1.1 | 1.1 | 1.7 |
| $^1$H | 1000        | 2.38 | 2.81 | 2.44 | 5.40 | 2.4 | 2.7 | 2.4 | 4.5 |
|      | 2000        | 6.47 | 8.12 | 6.91 | 15.94 | 6.4 | 7.7 | 6.9 | 15.0 |

For determination of mass resolution, the energy resolution at different incident energies was measured by backscattering experiment using a thin Au target. The mass resolution was then determined by equation (1) using the measured energy resolution. Figure 4 shows the dependences of obtained mass resolution as well as the energy resolution on the energy of $^4$He beam. It is seen from figure 4 that the energy resolution does not change when the energy of the incident beam increases and the corresponding obtained mass resolution decreases with the increase of energy of the incident beam. By using this procedure, one can determine the optimized energy of the incident beam in order to get the best mass resolution.

**Figure 4.** Experimental mass resolution (a) and corresponding energy resolution (b) as a function of energy of He ions.
The depth resolution for a specific energy of the beam and target tilting angle can be calculated by equation (3). For this purpose our simulation code provides an estimation of the stopping power and the total energy resolution that takes the energy resolution of the beam, the energy resolution of the detector and the energy straggling effect into account. The calculated values of the depth resolution were verified by backscattering experiment using a thin Au film at varying beam energies and target tilting angles. The uncertainty of the experimental values were less than 10.2%. Figure 5 shows the measured and calculated depth resolution at depth 200 x10^{15} atom/cm^2 for Au film as a function of the energy of the He beam and target tilting angles. For different beam energies, the measured depth resolutions are in agreement with the calculated values within 8.3%. The measured values for different tilting angles also fairly agreed with calculated value at the small angles up to 50 degrees. However, there are some noticeable discrepancies between measured and calculated values for large tilting angles. These discrepancies might be explained by the fact that the effects of large angle multiple scattering and lateral spreads were not included in the calculation. By using these obtained results we were able to choose the optimal beam energy as 1200 keV and the optimal target tilting angle of 50 degree.

![Graph](image)

**Figure 5.** Depth resolution at depth of 200x10^{15} cm^{-2} for Au sample as a function of the energy of the incident He ions in the case of target tilting angle of 50 degrees (a) and as a function of target tilting angles in the case of 2200 keV He ions (b).
The above optimization procedures were also successfully applied for a W implanted on Kapton sample having a depletion region of Oxygen caused by W layer. Two RBS spectra are presented in figure 6. The spectra on the left and right panels were obtained by using non-optimized and optimized experimental conditions respectively. It is seen from this figure that the mass resolution of the RBS spectrum with optimized experimental condition on the right side is better than that of non-optimized experimental condition.

Figure 6. The RBS spectra for the W implanted on Kapton sample using a non-optimized experimental condition (left) and an optimized experimental condition (right). The green marked region indicates effect of depletion of Oxygen from Kapton after implantation by a high dose of W

5. Conclusion
The dependences of the depth and mass resolutions of analysis using Rutherford Backscattering Spectrometry (RBS) on some experimental conditions (such as the beam energy, the target tilting angle, etc.) have been investigated. A computer program for simulating the RBS spectra and for calculating the depth and mass resolution under different experimental conditions was developed. The results of calculation were experimentally checked by using some reference samples. The good agreements between calculated and experimental values have been found. The optimum analysis conditions over a wide range of RBS applications based on our calculation can be chosen. This investigation was conducted by using the RBS system at HUS 5SDH-2 Tandem accelerator at the Hanoi University of Science. This work is supported by Hanoi University of Science.

Appendix

The energy resolution at surface of the sample in equation (1) is calculated as follows [12]

$$
\delta E_H = \left[ (\delta E_{BE})^2 + (\delta E_{BS})^2 + (\delta E_{BW})^2 + (\delta E_{SR})^2 + (\delta E_{AA})^2 + (\delta E_D)^2 \right]^{1/2}, \quad (A.1)
$$

where $\delta E_{BE}$ is the energy spread of the incident ion beam; $\delta E_{BS}$ is the angular spread of the incident ion beam; $\delta E_{BW}$ is the energy spread due to beam profile on the target; $\delta E_{SR}$ is due to the surface roughness of the sample; $\delta E_{AA}$ is due to the detector acceptance angle and $\delta E_D$ is the energy resolution of the detector. In our calculation only $\delta E_D$, $\delta E_{BE}$ and $\delta E_{SR}$ were considered. Therefore the energy resolution at a certain depth is given as

$$
\delta E_L = \left( \delta E_H^2 + \delta E_{ES}^2 + \delta E_{AS}^2 + \delta E_{LS}^2 \right)^{1/2}. \quad (A.2)
$$
The following formula was used to calculate the energy straggling $\delta E_{ES}$ of the incoming beam in solid

$$\delta E_{ES} = 2\left[2\ln2\right]^{1/2}\left(K^2\Omega_{in}^2 + \Omega_{out}^2\right)^{1/2},$$  \hspace{1cm} (A.3)

where $K$ is the kinematic factor. $\Omega_{in(out)}$ are calculated for incoming and outgoing path of the beam by using the well-known Bohr formula [7]

$$\Omega_{B} = 4\pi\left(Z_1e^2\right)^2Z_2Nt,$$  \hspace{1cm} (A.4)

where $Nt$ is the path length, $Z_1, Z_2$ the atomic number the projectile and the target, respectively.

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