Proceedings of ISINN-29, JINR, E3-2023-58, Dubna, 2023, p.159 –163

Using Rutherford Backscattering Spectroscopy to Investigate ErF_3 Doped CaF_2 Samples

P.L. Tuan[1,2,*], M. Kulik[3], M. Stef[4], T.V. Phuc[5,6], N.T.B. My[1,7], N.N. Anh[8,9], T.Y. Zelenyak[1], G. Buse[4], A. Racu[4], A. Doroshkevich[1], L.H. Khiem[5,6], V.D. Cong[1,5]

[1]*Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, 141980, Russia;*
[2]*Hanoi Irradiation Center, Vietnam Atomic Energy Institute, Hanoi, 129000, Viet Nam;*
[3]*Institute of Physics, Maria Curie-Skłodowska University, Pl. Marii Curie-Skłodowskiej 1, 20-031 Lublin, Poland;*
[4]*Faculty of Physics, West University of Timisoara, 300223 Timisoara, Romania;*
[5]*Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, 118500, Viet Nam;*
[6]*Graduate University for Science and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, 122100, Viet Nam;*
[7]*Institute for Nuclear Science and Technology, Vietnam Atomic Energy Institute, Hanoi, 122100, Viet Nam;*
[8]*Faculty of Fundamental Science, PHENIKAA University, Yen Nghia, Ha Dong, Hanoi 12116, Viet Nam;*
[9]*PHENIKAA Research and Technology Institute (PRATI), A&A Green Phoenix Group JSC, No.167 Hoang Ngan, Trung Hoa, Cau Giay, Hanoi 11313, Viet Nam.*

Rutherford backscattering spectroscopy (RBS), a nuclear method, was used to study ErF_3 doped CaF_2 samples at varied concentrations. The acquired results allow us to determine the linked changes in the element concentrations of the samples as Er^{3+} ions are doped. Furthermore, we construct the model using the SIMNRA computer code to simulate the RBS spectra of all the studied samples with varying incidence angles. We may use the model to determine the depth profile of elements obtained directly from the RBS experiment spectra because the simulated spectra correspond well with the experimental spectra.

Keywords: RBS; SIMNRA; depth profile; calcium fluoride;

**Corresponding author: phanluongtuan@gmail.com*

1. Introduction

Rutherford backscattering spectroscopy (RBS) is based on the principles of elastic scattering, which were first discovered by Ernest Rutherford in the early 20th century. Rutherford conducted his famous gold foil experiment, in which he bombarded a thin gold foil with alpha particles and observed their scattering patterns [1]. This experiment led to the discovery of the atomic nucleus and provided the foundation for RBS. Over the years, RBS has undergone continuous refinement and improvement. The advent of accelerator technology with the availability of high-energy ion beams and sophisticated detectors, such as silicon surface barrier detectors [2] and position-sensitive detectors, enabled more accurate and precise measurements of the backscattered particles [3]. These advancements facilitated the analysis of thinner films and provided a deeper understanding of surface layers and interfaces. In addition to technological advancements, the development of computer algorithms and

modeling techniques has played a vital role in the progress of RBS. Theoretical models and simulations have been developed to interpret the experimental data, allowing researchers to extract detailed information about the sample, such as elemental depth profiles and film thicknesses [4,5]. Today, RBS has become a powerful analytical technique in materials science, semiconductor industry, and nuclear physics research. It is a non-destructive method used to investigate the composition and structure of thin films and surfaces [6].

In this study, we investigate ErF_3 doped CaF_2 samples using the RBS method. To accomplish this, the samples were produced with varying concentrations of ErF_3. The RBS examines were conducted with varying incident angles to investigate the depth profile of elements in the samples. SIMNRA computer code was used to build the model, which was used to determine the concentration and depth distribution of elements in the samples.

2. Rutherford backscattering spectroscopy (RBS)

RBS is based on the elastic scattering of high-energy ions (usually helium or hydrogen) from the nuclei in a sample. RBS is unique in that it allows quantification without the use of reference standards. The RBS can determine elemental composition, atomic concentration, depth distribution of elements in samples. A detailed explanation of the basic concepts behind the RBS approach was provided in [1] and the following is a brief introduction. Fig. 1 shows the backscattering process schematic.

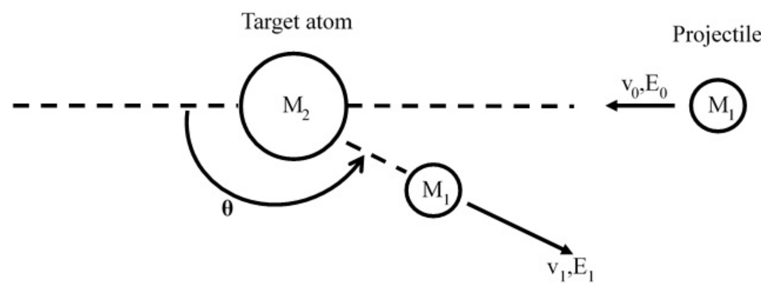

Fig. 1: Graphic illustrating an elastic collision between a projectile with mass M_1, velocity v_0, and energy E_0 and a resting target mass M_2.

A stationary particle of mass M_2 collides elastically with an incoming ion of mass M_1 traveling at v_0 and with kinetic energy E_0. Following collision, the incident ion moves with a velocity of v_1 and kinetic energy of E_1 at a scattering angle of θ with regard to the incident direction. The kinematic factor K, which depends on the mass of the incident ion M_1, mass of the scattered particle M_2, and the scattering angle θ, is the ratio of the kinetic energy after a collision to the kinetic energy before a collision.

$$K = \frac{E_1}{E_0} = \frac{M_1.v_1^2}{M_2.v_0^2} = \left(\frac{M_1.cos\theta + \left(M_2^2 - M_1^2.sin^2\theta\right)^{1/2}}{M_1+M_2}\right)^2 \quad (1)$$

If E_0, M_1, and θ are known, one may use this method to calculate M_2 by measuring the energy E_1 following a collision. The RBS method gives an option for determining the atomic mass of elements in samples with kinematic factor K. The differential scattering cross section $\frac{d\delta}{d\Omega}$ with the solid angle of detection Ω gives the likelihood that a collision will produce a detected particle. Rutherford's formula yields the cross section for differential scattering:

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{2E}\right)^2 \cdot \frac{\left\{cos\theta + \left[1 - \left({}^{M_1}/_{M_2} sin\theta\right)^2\right]^{1/2}\right\}^2}{sin^4\theta\left[1 - \left({}^{M_1}/_{M_2} sin\theta\right)^2\right]^{1/2}} \quad (2)$$

Only when $M_1 << M_2$ does this formula hold true for values in the laboratory frame of reference. This equation makes $\frac{d\delta}{d\Omega}$ proportional to Z_2^2. Heavy atoms scatter light atoms far more effectively than light atoms do for any given projectile. So, compared to light elements, RBS is considerably more sensitive to them. A typical surface-barrier detector system in RBS has a solid angle Ω that is rather small and could be referred to as a differential solid angle $d\Omega$. The average differential scattering cross section, often known as the scattering cross section σ, is then conveniently introduced:

$$\sigma = \left(\frac{1}{\Omega}\right) \cdot \int_\Omega \left(\frac{d\sigma}{d\Omega}\right) d\Omega \quad (3)$$

With very small detector angle Ω, $\sigma \rightarrow \frac{d\delta}{d\Omega}$

In the experimental setup, a uniform beam is incident on a uniform target at normal incidence. The target is bigger than the region covered by the beam. The total number of detected particles, denoted as A, can be expressed as:

$$A = \sigma\Omega \cdot Q \cdot Nt \quad (4)$$

This equation demonstrates that the number of atoms per unit area in the target (elements composition), Nt, may be calculated when σ and Ω are known and the number of incident and detected particles are tallied. The additional energy loss that occurs as the beam enters and exits the target can be used to estimate the depth of a specific type of nucleus. The depth of penetration of the beam depends on its initial energy.

3. Experiments

The preparation of ErF_3 doped CaF_2 samples with different concentration was conducted at West University of Timisoara, Romania utilizing the vertical Bridgman method [7]. The RBS measurements were carried out at the Frank Laboratory of Neutron Physics (FLNP), Joint Institute for Nuclear Research (JINR), Dubna, Russia. The operating pressure in the scattering chamber was less than 10^{-4} Pa. The samples were put on the holders which is possible to change the incident angle continuously without breaking vacuum. To investigate the depth profile of elements in the samples, the various incident angles at 30^0 and 0^0 were applied. The diameter of α-beam with energy 2 MeV, which was generated by EG5 Van de Graff accelerator, is 1 mm. The silicon planar detector with 15 ÷ 25 keV energy resolution was placed at the scattering angle of 170^0 away from the beam incident direction. The solid angle of the particle detector was 0.002 sr. More details connected with the RBS experimental setup were reported in [4,5] The calculated spectra have been derived with the help of the SIMNRA computer code [8].

4. Results and discussions

The spectra from RBS experiments are presented in Fig. 2 for the samples with different concentration of ErF_3 doped CaF_2.

We have identified three kinematic borders in the spectra, which are located close to channels 800, 600, and 400. The energy of He^+ ions backscattering on Er atoms at the surface layer of the samples is indicated by the kinematic border around channel number 800. The Er

concentration in the samples is correlated with the height of the Er signal in the region between channels 600 and 800. The energy of He^+ ions backscattering on Ca and F nuclei in the samples is shown by the other kinematic limits close to channels 600 and 400.

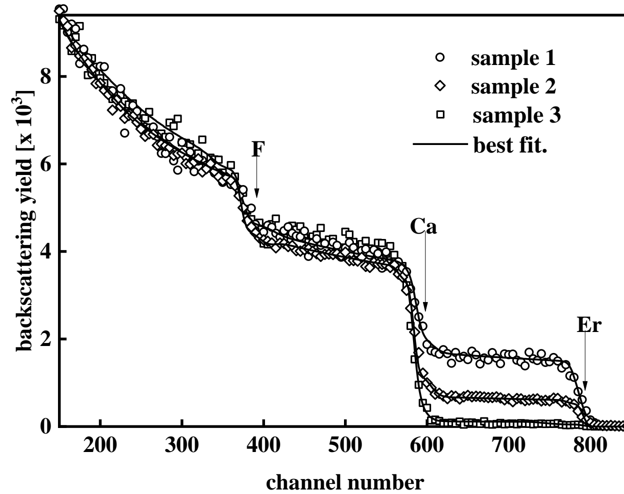

Fig. 2: RBS spectra collected from ErF_3 doped CaF_2 samples.

The depth profile of the samples under investigation is studied using the SIMNRA computer code. The computer code can simulate the RBS spectrum of a sample model that the user has defined. The program includes all experimental details, such as detector resolution, energy per channel, incidence angle, and scattering angle. Users must provide SIMNRA with identical replicas of the detector and ion beam specifications used in the investigations. The sample structure information is also known as the sample model. In particular, the model allows for the examination of the sample's depth profile by allowing for the division of the model into numerous layers. A four-layer model was used in this investigation. The element concentrations of Ca, F, and Er are among the model parameters for each layer. These model parameters are adjusted until the simulated and observed RBS spectra agree. In Table 1, the thickness and elemental makeup of the models are displayed.

Table 1: Depth profiles of all elements are contained in the CaF_2:ErF_3 samples

The models	**Layers**	**Thickness (10^{15} atoms/cm^2)**	**atomic concentration (%)**		
			F	**Ca**	**Er**
Sample 1	1	4000	66.50	31.50	2.00
	2	5000	66.30	31.70	2.00
	3	4000	66.29	31.71	2.00
	4	6000	66.30	31.70	2.00
Sample 2	1	4000	65.50	33.82	0.68
	2	6000	65.00	34.30	0.70
	3	3000	65.02	34.28	0.70
	4	5000	64.99	34.31	0.70
Sample 3	1	6000	61.93	38.00	0.07
	2	5000	62.00	37.93	0.07
	3	6000	62.03	37.90	0.07
	4	7000	62.01	37.92	0.07

5. Conclusion

RBS is a non-destructive method that can provide in-depth knowledge on the distribution and composition of elements in a material. This investigation's goal is to assess the RBS-mediated incorporation of ErF_3 into CaF_2 samples. The results of this study can help improve our understanding of the atomic-scale interactions between ErF_3 and CaF_2 while also shedding light on doped samples. The model was successfully built using the SIMNRA computer code, and it offers detailed data on the distribution and elemental composition of the samples.

Acknowledgments

The authors wish to acknowledge the technical staff of the EG-5 group, FLNP, JINR for the RBS measurements. The study was performed in the scope of RO-JINR Project No. 366/2021 item 84, and Vietnam-the International Center of Physics at the Institute of Physics Grant ICP.2022.04.

References

1. W.K. Chu, J.W. Mayer, and M.A. Nicolet, Backscattering Spectroscopy, Academic Press, New York, 1978.
2. Kim HS, Park SH, Ha JH, Cho SY, Kim YK. Characteristics of Silicon Surface Barrier Radiation Detectors for Alpha Particle Detection. JKPS 2008; 52:1754-1758. https://doi.org/10.3938/jkps.52.1754.
3. Grupen, C., & Shwartz, B. (2008). Particle Detectors (2nd ed., Cambridge Monographs on Particle Physics, Nuclear Physics and Cosmology). Cambridge: Cambridge University Press. doi:10.1017/CBO9780511534966
4. T.V. Phuc, M. Kulik, D. Kołodyńska, L.H. Khiem, P.L. Tuan, J. Zuk, M. Turek, Investigations of chemical and atomic composition of native oxide layers covering SI GaAs implanted with Xe ions, Surface and Coating Technology 387 (2020). doi.org/10.1016/j.surfcoat.2020.125871.
5. P.L. Tuan, M. Kulik, J. Nowicka-Scheibe, J. Zuk, P. Horodek, L.H. Khiem, T.V. Phuc, Nguyen Ngoc Anh, M. Turek, Investigations of chemical and atomic composition of native oxide layers covering SI GaAs implanted with Xe ions, Surface Coating. Technol. 394 (2020), doi.org/10.1016/j.surfcoat.2020.125871
6. Nastasi, M., Mayer, J.W., & Wang, Y. (2014). Ion Beam Analysis: Fundamentals and Applications (1st ed.). CRC Press. doi.org/10.1201/b17310
7. I. Nicoara, M. Stef, Growth and Characterization of Doped CaF2 Crystals, Modern Aspects of Bulk Crystal and Thin Film Preparation, InTechOpen (2012). DOI: 10.5772/28943.
8. M. Mayer, SIMNRA User’s Guide, Max-Planck-Institut fur Plasmaphysik, Garching, Germany.