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CALCULATION AND OPTIMIZATION OF EXPERIMENTAL PARAMETERS IN ELASTIC RECOIL DETECTION (ERD)

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ABSTRACT

Elastic recoil detection (ERD) proposed for the analysis of light elements in a heavier matrix is an appropriate method for its specialities. Optimization of experimental parameters in ERD such as scattering geometry and incident beam energy is very important when using a small accelerator with energy lower than 10 MeV. In this paper a computer program ERDA1 is developed for the purpose, and is proved to be useful for practical handling of ERD experiments.

Key words: Elastic recoil detection Maximum detectable depth Depth resolution

Ⅰ. INTRODUCTION

The properties of solid surface are remarkably changed by the presence of any light element ranging from hydrogen to oxygen. Analysis and detection of light elements distributions in solids are interesting problems and useful tools in many research fields such like the study of ion beam technique, hydrogen and helium embrittlement in metals, solar cells, semiconductor industry, superconducting materials, fusion reaction materials, etc., and has attracted much attention in the past ten years or so[3,4].

L'Ecuyer et al.,[1] proposed the use of elastic recoil detection for analysis and depth profiling of light elements in near surface regions of solids. Satisfactory depth resolution, time saving, nondestruction and simultaneous detection of various impurities are the merits of this method[2].

The depth distribution of specimens of hydrogen[5,6] or helium[7] implanted in silicon were detected successfully. A small tandem accelerator with the incident beam of $^{19}F^{3+}$ was used, and the depth resolution of 20– 40 nm was obtained. For ERD method, it is necessary to know the optimal experimental parameters such as the incident ion species, the beam energy, the scattering geometry and the thickness of absorber, etc.. All these parameters must be determined thoroughly before the performance of an experiment, especially for experiments at energy lower than 10 MeV. Otherwise, the risk of failure of the experiment is high. Therefore, it is desirable to develop a computer program for designing ERD experiment and selecting the optimal parameters in advance. The ERD experimental set-up and skill are described in Ref.[6].

To this end, a computer program called ERDA1 is written for the calculation of the maximum detectable depth, the depth resolution, the total energy resolution, the recoil spectrum energy of light element to be analyzed and the thickness of the absorber. This is achieved by considering the operating specifications of the small tandem accelerator, choosing one of the ion beams of Li^{+n}, C^{+n}, O^{+n}, F^{+n}, Cl^{+n}, which are frequently used in the routine analyses, using different scattering geometry and designing optimal experimental parameters.

Ⅱ. COMPUTER PROGRAM FOR OPTIMIZATION

Computer program ERDA1 is based on the principle of elastic recoil scattering[6-8]. It is simular to the backscattering but in different counting geometry. In this section, depth resolution and maximum detectable depth are described in detail. Depth resolution means the distance between two thin slabs at depth x within a target, corresponding to the energy interval on the spectrum of two Gaussian peaks which are just distinguishable by the detecting system. So, it is determined by the total energy resolution δE of the analyzing system. $Y(E)$ is the theoretical yield, where E is the energy, if energy spread δE is taken into account, the yield of actual spectrum is expressed as

$$Y_0(E) = \int_0 Y(w)\,[1/(1.06\delta E)\; e^{[-(w-E)^2/0.36\delta E^2]}\, dw \qquad (1)$$

and the depth resolution is expressed as:

$$\delta x = \delta E\,(\triangle x/\triangle E) \qquad (2)$$

where $\triangle x/\triangle E$ is decided by the stopping power. The evaluation of depth resolution for ERD method is made by calculating separately the energy spred due to various contributions. The total energy resolution is determined by many factors, such like the energy straggling of ions in target and absorber foil, the geometrical broadening of beam spread and detector, the multiple scattering and the detector resolution. The total energy resolution is [8]:

$$\delta E = [\delta E_d^2 + \delta E_g^2 + \delta E_{si}^2 + \delta E_{so}^2 + \delta E_{sf}^2 + \delta E_{ms}^2]^{1/2} \qquad (3)$$

The meaning of various terms in Eq.(3) are listed below:

1. dE_d is the detector resolution.

2. dE_θ is the energy spreading of geometrical contribution arising from the finite detector acceptance angle and energy dispersion of the incident beam.

$$\begin{aligned} \delta E_g &= [E_1(dk/d\theta) + (E_2 - E_3)\,\mathrm{ctg}\,(\theta - \alpha)]\,\delta r \\ \delta r &= (s^2 + d^2 \sin^2(\theta - \alpha))^{1/2}/D \end{aligned} \qquad (4)$$

where E_1 is the energy just before the collision at depth x in the target; E_2 is the recoil energy just after collision; $E_2 = K \times E$, K is the kinematic factor of elastic recoil; E_3 is the energy of recoil particles emerging from the surface of the target; E_f is the detected energy; α is the incident angle and θ is the recoil angle; s is the diameter of the detector aperture; d is the incident beam width in the scattering plane and $d = WB/\sin\alpha$, where WB is the incident beam diameter; D is the distance between detector and target.

3. dE_{si}, dE_{so}, dE_{sf} are the energy stragglings of the incident beam in target, the recoil particles in target and in absorber respectively, and are expressed by:

$$\delta E_{si} = K\, 4Z_1 e^2 (2\pi \ln 2 Z_T N_T x/\sin\alpha)^{1/2} \tag{5}$$

$$\delta E_{so} = 4Z_D e^2 [2\pi \ln 2 Z_T N_T x/\sin(\theta - \alpha)]^{1/2} \tag{6}$$

$$\delta E_{sf} = 4Z_D e^2 (2\pi \ln 2 Z_f N_f t_f)^{1/2} \tag{7}$$

where x is the depth in target; t_f is the thickness of the absorber; N_T, N_f are the atomic densities of the target and the absorber respectively, Z_1, Z_D, Z_T, Z_f are the atomic numbers of the incident beam, the light impurity, the target and the absorber respectively.

4. dE_{ms} is the energy spread of angular spread and lateral spread caused by multiple scattering[8-9], and is expressed by:

$$\delta E_{ms} = K\,[E_1(dk/d\theta) + (E_1 - E_0)p\,ctg\alpha]\varphi_{in} + [KE_1(dk/d\theta) + (E_2 - E_3)p\,ctg(\theta - \alpha)]\varphi_{out} \tag{8}$$

$$p = 0.4285$$

$$\varphi_{in} = [0.6667 Z_T Z_1 x/\sin\alpha]/[(Z_T^{2/3} + Z_1^{2/3})^{1/2} E_{in}]$$

$$\varphi_{out} = [0.6667 Z_T Z_1 x/\sin(\theta - \alpha)]/[(Z_T^{2/3} + Z_1^{2/3})^{1/2} E_{out}]$$

where E_{in}, E_{out} are the incoming and outgoing energy respectively.

It is known from Ref.[6], that heavy recoil particles of target or other elements and scattered ions of incident beam are eliminated by stopping them in an absorber of appropriate thickness. The stopping of the scattered beam ions is difficult and can only be accomplished— without also stopping the light impurity ions— if it is much heavier than the light impurity atoms. The heavy recoil particles of target will also be stopped because of its mass is always heavier than the incident ions. So, a clear recoil spectrum of light impurity element is obtained from MCA. In this computer program, the thickness of absorber is calculated first. Scattered from the target surface, beam ions with energy $K_R \times E_0$ (K_R is the kinematic factor of Rutherford scattering) penetrate into the absorber foil perpendicularly and loss their energy. Divide the foil into several thin sublayers, the energy and energy stopping of every sublayer can be calculated by iteration. Scattered beam ions pass through the stopping foil until the whole energy is exhansted and the ions are stopped. The marginal thickness of the foil t_f is the thickness to be calculated.

The target is subdivided into many thin slabs in depth too. For a given subslab— say the i—th slab in depth $X(i)$ in target—the energies $E_1(i)$, $E_2(i)$, $E_3(i)$ and $E_f(i)$ are calculated by the subroutines of stoppings and an iterative subroutine of the computer program. Calculating E_1, E_2, E_3 ,E_f step by step for every sublayer, the corresponding curves of these energies versus depth x are obtained. The factor $\triangle x/\triangle E$ of formula (2) can be evaluated. Each contribution of energy spread in formulas (4) to (8) are calculated by those energy vs. depth x relations and other parameters corresponding to a given system. Then substitute these values to formulas (3) and (2), the total energy resolution and the depth resolution are obtained. Energy $E_f(i)$ is namely the same detected energy in the spectrum of MCA, corresponding to the recoil signal of depth $X(i)$ in target. When $i=j_0$, *if* $E_f(j_0) = E_{cho}$, where E_{cho} is the energy of the zero channel of MCA, the depth of the j_0-th sublayer $X(j_0)$ is the maximum detectable depth.

In this computer program, the subroutines of stopping power calculation and data files are taken from software[10]. Source files of the program are written in FORTRAN-IV and contain about 600 statements. It is applicable for IBM-PC-XT microcomputers.

Ⅲ. RESULTS AND DISCUSSIONS

For different matrices and light element impurities, selection of the incident species, the beam energy, the scattering geometry and absorber foil thickness is very important in ERD experiments. By the use of this program ERDA1, optimization could be done easily. As an example, the calculation of the optimal conditions for the analysis of He in Si is discussed. The incident ions and absorber are selected to be fluorine ions and aluminium foil respectively, and the calculating parameters are: E_0 from 4 MeV to 10 MeV, α from 5° to 25°, θ from 18° to 42°, $dE_d = 17$ keV, $s=3$ mm, $WB=1$ mm and $D=70$ mm.

1. Calculation of absorber thickness t_f

The relations between t_f and E_0 are indicated in solid lines in Fig.1 with three values of θ . It is linear. For aluminium foil, with the incident energy increased by 1 MeV, the increase of the foil thickness is about 0.6μ m.

2. Calculation of detectable depth

The curves of maximum detectable depth X_{max} versus incident energy are shown in Fig.1 in broken lines for various recoil angles θ and in Fig.2 for various incident angles α . With increasing incident energy E_0 the maximum detectable depth is increased obviously. The curves of maximum detectable depth X_{max} vs. incident angle α are roughly parabola in Fig.3 and the maximum value is close to $\alpha = 20°$. And it can be seen in Fig.1 and Fig.3, that the maximum detectable depth at recoil angle $\theta = 30°$ is better than that at $\theta = 18°$ and 42°.

3. Calculation of depth resolution

Depth resolution δ x versus depth x relations at different incident energies and angles are shown in Fig.4 and Fig.5. The terminal of each curve is the maximum

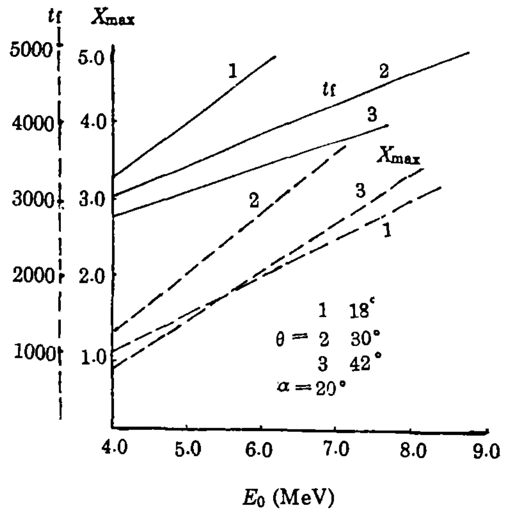


Fig.1 Curves of maximum detectable depth X_{max} vs. incident energy E_0

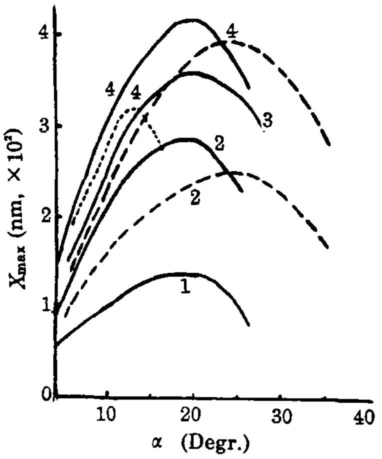
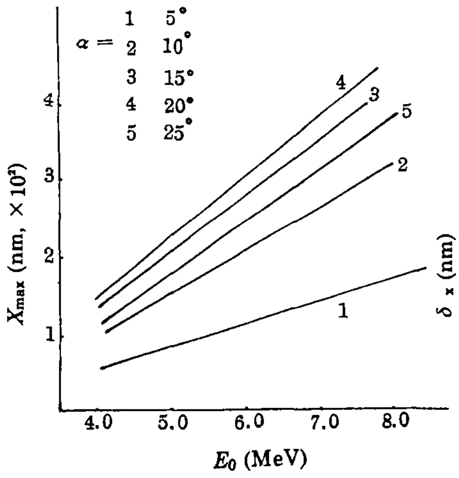


Fig.2 Curves of X_{max} vs. incident angle α for different θ and E_0

E_0 = 1, 4 MeV 2, 6 MeV
3, 6.8MeV 4, 7.5MeV
θ = · 30°
-- 42°
—— 18°



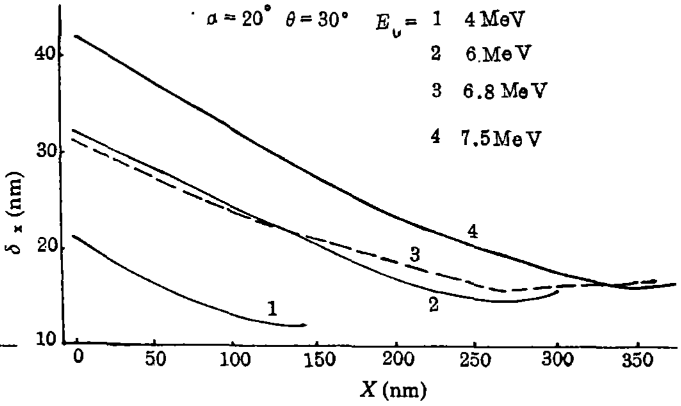


Fig.3 Depth resolution δ_0 vs. depth X curves for different α at E_0= 6 MeV and θ = 30°

Fig.4 Depth resolution δ_x vs. depth xcurves for different E_0 at α = 20° and θ = 30°

detectable depth under a given condition. Depth resolution δ x is improved with decreasing incident energy E_0, but lower energy will diminish the probing depth, so it is not advised to decrease the incident energy. At the first sight, in the very surface region of the sample the depth resolution seems to be good for $\alpha < 10°$ or $\alpha > 25°$, however the rapid change at the deeper depth for $\alpha = 25°$, and short probing depth at both 10° and 25° indicate that they are not satisfactory. When α equals to 10°, 15° and 20°, the calculated relations of depth resolution vs. depth x are quite flat which allow a considerable detectable depth and depth resolution. Incident angle is a very sensitive parameter. With the results of calculation, using F^{3+} ions at energy lower than 10 MeV as an analyzing beam, if $\alpha = 20°$ and $\theta = 30°$ the depth resolution is about 30 nm to 40 nm and the detectable depth reaches 300 nm. This computer program efficiently helps experiment design.

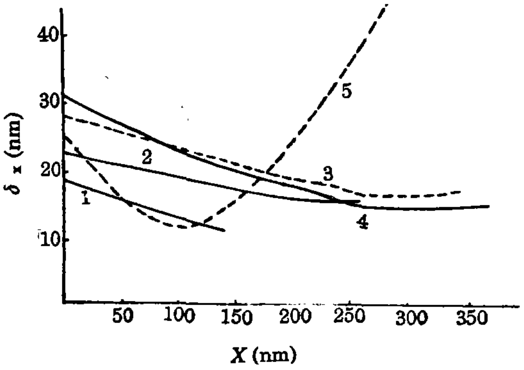


Fig.5 Depth resolution δ x vs. depth x curves for different E_0 at $\alpha = 20°$ and $\theta = 30°$
Curve 1 for $E_0 = 4$MeV, 2 for 6MeV, 3 for 6.8MeV, 4 for 7.5MeV.

Recently, the time of flight (TOF) mode ERD method[11] improves the detection and profiling. The TOF mode ERD method does not need an absorber, so both depth resolution and maximum detectable depth are improved. Furthermore, because this method has no problems of the mass spectrum overlapping, so simultaneous detection of various impurities are more desirable. Development of TOF mode for ERD method and analysis is in progress in our laboratory.

REFERENCES

[1] J.L'Ecuyer et al., *J. Appl. Phys.*, **47** (1976), 381.
[2] B.Terreault et al., *J. Vac. Sci. Tech.*, **14** (1977),1:492.
[3] J.L'Ecuyer et al., *Nucl. Instr. Meth.*, **149** (1978), 271.
[4] B.L.Doyle and P.S.Peercy, *Appl. Phys. Lett.*, **34** (1979), 811.
[5] J. Liu et al., *Chinese Phys. Lett.*, **4** (1987),6:249.
[6] J. Liu et al., *Acta Physica Sinica*, **37** (1988), 1 : 71.
[7] P.Zhu et al., Nucl. Sci. Tech., 1 (1990).
[8] A.Turos and O.Meyer, *Nucl. Instr. Meth.*, **B4** (1984), 92.
[9] A.D.Marwick et al., *Nucl. Instr. Meth.*, **126** (1975), 317.
[10] J.F.Ziegler et al., The stopping and ranges of ions in solids, N.Y., 1985, p.202.
[11] J.P.Thomes et al., *Nucl. Instr. Meth.*, **B15** (1986), 443.