Range straggling and lateral spread of MeV Au⁺ ions in LiB₃O₅ and SiN_{1.375}H_{0.603}

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Abstract. Both LiB₃O₅ and SiN_{1.375}H_{0.603} were implanted by 1.0 MeV Au⁺ ions to a dose of 5×10^{15} ions cm⁻² under different angles. The range straggling and lateral spread of 1.0 MeV Au⁺ ions in both LiB₃O₅ and SiN_{1.375}H_{0.603} were investigated by the Rutherford backscattering of 2.1 MeV He²⁺. The experimental mean projected range, range straggling and lateral spread are 279.7 nm, 54.0 nm and 34.6 nm for the case of LiB₃O₅, and 222.3 nm, 54.6 nm and 31.5 nm for the case of SiN_{1.375}H_{0.603}. The results show that the experimental range straggling and lateral spread are much larger than the values predicted by the 1998 version of the Transport of Ions in Matter code (TRIM98). After inelastic effects have been included in nuclear stopping regime, there is a much closer agreement with the experimental values than the original TRIM98 codes have. The maximum differences of the mean projected range, range straggling and lateral spread between experimental and calculated values are less than 3%, 24% and 21%, respectively for both cases.

1. Introduction

The knowledge of the slowing down of ions in traversing matter is of fundamental importance in ion beam analysis and material modification. The physics of energy loss phenomena is very complex, involving many kinds of interactions between the projectile ion, target nuclei and target electrons. Because of their significance in many fields of physics, these phenomena have been subjected to intense studies since the beginning of this century [1]. The Transport of Ions in Matter, version 1998 (TRIM98) code has been used extensively to predict the range parameters [2, 3]. With ion implanted devices being developed with smaller dimensions, precise information is needed not only for the depth distribution of the implanted ions along the surface normal, but also for their distributions perpendicular to the surface normal, which are governed essentially by the lateral spread [4].

In the present work, the range straggling and lateral spread have been measured by the Rutherford backscattering technique for 1.0 MeV Au⁺ implanted into LiB₃O₅ and SiN_{1.375}H_{0.603} and have then been compared with the TRIM98 predictions.

Lithium triborate (LiB₃O₅) is an attractive material for frequency up conversion of visible radiation to the UV light because of its high UV transmission, large acceptance angle, small walk-off angle, good chemical stability, nonhygroscopicity and high frequency doubling

efficiency. But its moderate effective nonlinear coefficient has limited its use for the harmonic generation of a high-power laser beam [5]. The waveguide formation in LiB₃O₅ makes it possible to extend its practical use to lower power lasers [6]. Davis *et al* [7] have reported the planar waveguide fabrication in LiB₃O₅ by ion implantation. Similarly, thin films of amorphous hydrated silicon nitride α -SiN_xH have several applications in microelectronic devices, including interlayer dielectrics, passivation layers, and as a gate dielectric in thin-film transistors [8]. During the last few years, different groups have performed systematic studies of the mean projected range and range straggling for several ions implanted into different substrates [9]. They found that, overall, a close agreement (around 10%) is observed when these data are compared with the TRIM98 calculations of the mean projected range. The experimental range straggling is usually higher than the TRIM98 prediction. But the energy region concerned is usually less than 400 keV and the target is usually a mono-elemental one, such as Si. Reports on the study of the range straggling and lateral spread of MeV ions implanted into Si as well as a polyatomic target are few [10–12].

2. Experimental details

The LiB₃O₅ crystals were obtained from the Institute of Crystal Materials, Shandong University. The samples, with

a density of 2.47 g cm^{-3} , were cut along the z direction and optically polished yielding a surface of $6 \times 6 \text{ mm}^2$. In an attempt to avoid accident channelling, the sample was tilted by 7° off the incident beam direction instead of normal incidence. The 1.0 MeV Au^+ ions were implanted into the samples to a dose of $5 \times 10^{15} \text{ ions cm}^{-2}$. In order to obtain the lateral spread, tilt angle implantations have been performed at 45° and 60° . The $\text{SiN}_{1.375}\text{H}_{0.603}$ films, having a density of 3.1 g cm^{-3} , were provided by the University at Albany, USA. The composition of the $\text{SiN}_{1.375}\text{H}_{0.603}$ film was determined by Rutherford backscattering and $\text{H}(^{15}\text{N}, \alpha)^{12}\text{C}$ nuclear reaction. Similarly, 1.0 MeV Au^+ ions were implanted into $\text{SiN}_{1.375}\text{H}_{0.603}$ at 0° , 45° and 60° angles to a dose of $5 \times 10^{15} \text{ ions cm}^{-2}$. The beam current density was 100 nA cm^{-2} . The power loading was 0.1 W . The temperature of the target during implantation was less than 60°C . The possible loss of hydrogen from the $\text{SiN}_{1.375}\text{H}_{0.603}$ film during implantation has not been measured by nuclear reaction.

The depth distributions were measured by the Rutherford backscattering of 2.1 MeV He ions. The backscattered He particles were detected by an Au(Si) barrier detector placed at 165° with respect to the beam direction. A gold film was used to calibrate the Au surface position of the energy spectra.

Different distribution functions have been presented to fit the experimental data of the depth profiles of ions implanted into solids [13]. In the present work, we are interested in the study of the range straggling and lateral spread of 1.0 MeV Au^+ ions implanted into both LiB_3O_5 and $\text{SiN}_{1.375}\text{H}_{0.603}$. The third and fourth moments of depth profile are not important; we have used a Gaussian function to fit the experimental data.

The MeV ion implantation was carried out at the 1.7 MV tandem accelerator of Peking University. The Rutherford backscattering measurement was performed at the 1.7 MV tandem accelerator of Shandong University.

3. Results and discussion

Figure 1 shows the depth distribution of the 1.0 MeV Au^+ ions implanted into LiB_3O_5 obtained by the Rutherford backscattering of 2.1 MeV He ions. The circles represent the experimental data. The full curve, which represents the Gaussian fit to the data, shows that the implanted Au distribution is nearly Gaussian in shape. The energy-to-depth transformation was done using the He stopping cross-section [14]. In the present calculation, we assume that Bragg's rule is valid [15]. The accuracy of Bragg's rule is limited, but for compound targets and heavy ion beams, many experiments have shown that the deviations from Bragg's rule become insignificant [16]. The experimental mean projected range R_p is 279.7 nm . The range straggling ΔR_p is related to the FWHM (full width at half maximum) of the Gaussian distribution via the formula: $\Delta R_p = \text{FWHM} / 2.355 N[\varepsilon]$ where N is atomic density of material and $[\varepsilon]$ is the stopping cross-section factor. From the measured FWHM, it is necessary to deconvolute the system resolution and energy straggling of He ions [17]. There are no experimental data of the He ion energy straggling in LiB_3O_5 ; we have estimated it using [18]. The range straggling obtained is 54.0 nm while the corresponding TRIM98 predicted value is 33.6 nm .

Figure 1. The depth distribution of 1.0 MeV Au^+ implanted into LiB_3O_5 (LBO) at a tilt angle of 7° . The circles represent the experimental data. The full curve represents the Gaussian fit.

Figure 2. The depth distribution of 1.0 MeV Au^+ implanted into LiB_3O_5 (LBO) at a tilt angle of 45° and 60° . The open circles and full squares represent the experimental data for 45° and 60° implantation, respectively. The full curves represent the Gaussian fits.

Figure 2 shows the depth distribution of 1.0 MeV Au^+ implanted into LiB_3O_5 at tilt angles of 45° and 60° . The open circles and full squares represent the experimental data at 45° and 60° while the full curves represent the Gaussian fits. The agreements suggest a nearly Gaussian profile for the depth distributions. According to the report by Furukawa and Matsumura [19], the lateral spread can be estimated using the tilt angle implantation data. If the spatial probability distribution of the deposited ions is a three-dimensional Gaussian, then the depth distribution in a target tilted at an angle θ to the incident ion beam also becomes a Gaussian with a standard deviation ΔD . The following relation holds:

$$(\Delta D)^2 = (\Delta R_p)^2 \cos^2 \theta + (\Delta X)^2 \sin^2 \theta$$

where ΔX is the lateral spread which can be estimated from

Figure 3. The depth distribution of 1.0 MeV Au^+ implanted into $\text{SiN}_{1.375}\text{H}_{0.603}$ (SiNH) at 0° and 45° . The open and full circles represent the experimental data for 0° and 45° implantation, respectively. The full curves represent the Gaussian fits.

the measurement of ΔD at a different angle θ . The true value of ΔD could be extracted from the measured deviation value considering the energy resolution of the measuring system and energy straggling of He ions. The lateral spreads obtained for 1.0 MeV Au^+ implanted into LiB_3O_5 are 33.0 nm and 34.2 nm from the sets of 7° and 45° , respectively, as well as 7° and 60° . The mean value of the lateral spread is 33.6 nm. The deviation from the mean value is less than 2% for the two measurements. The calculated lateral spread ΔX by TRIM98 is 23.1 nm which is much lower than the experimental value.

Figure 3 shows the depth distributions of 1.0 MeV Au^+ implanted at 0° and 45° into $\text{SiN}_{1.375}\text{H}_{0.603}$ to a dose of 5×10^{15} ions cm^{-2} . The circles represent the experimental data. The full curves represent the Gaussian fits. Again the depth distribution is nearly Gaussian in shape. The mean projected range is 222.3 nm. The experimental range straggling ΔR_p is 54.6 nm. The calculated value by TRIM98 is 34.6 nm. The experimental lateral spread is 29.8 nm while the TRIM98 calculated value is 24.0 nm. Again the experimental values of the range straggling and lateral spread are significantly larger than the calculated ones.

Figure 4 shows the depth distributions of 1.0 MeV Au^+ implanted at 0° and 60° into an $\text{SiN}_{1.375}\text{H}_{0.603}$ film. The depth distributions are still nearly Gaussian in shape, as can be seen from the excellent fits. Note that the peak position of the implanted Au^+ depth distribution shifts toward the surface with the increase of the angle θ , and the FWHM gets narrower. The lateral spread is 33.2 nm for the set of 0° and 60° . The average value of the lateral spread is 31.5 nm for sets of 0° and 45° as well as 0° and 60° . The deviation from the mean value is less than 5% for both measurements. Again the experimental lateral spread is significantly larger than the value calculated using TRIM98.

Table 1 summarizes the comparison of the experimental values with the calculated values for the mean projected range, the range straggling and lateral spread in the case

Figure 4. The depth distribution of 1.0 MeV Au^+ implanted into $\text{SiN}_{1.375}\text{H}_{0.603}$ (SiNH) at 0° and 60° . The open and full circles represent the experimental data for 0° and 60° implantation, respectively. The full curves represent the Gaussian fits.

of LiB_3O_5 and $\text{SiN}_{1.375}\text{H}_{0.603}$. These results are somewhat similar to those reported by Behar *et al* [3] for Au^+ and Bi^+ implanted into photoresist films. It is found that the experimental data significantly deviate from values calculated by TRIM98. The possible reasons are as follows:

- (1) the error in the calculation of the energy-loss to depth transformation is due to the reported uncertainty in the He particle stopping power;
- (2) in the present work, the statistical errors estimated in the projected range, range straggling and lateral spread are less than 1%, 5% and 5%, respectively;
- (3) the possible modification of nominal composition—in [3] it was reported that a reasonable modification of nominal composition (around 10% for each component) gives a variation of only 2% to 5% in the theoretical–experimental discrepancies;
- (4) in the present TRIM98 code, there is no correlation between the nuclear and electronic stopping power.

The ZBL (Ziegler, Biersack and Littmark) calculations are performed under the usual simplified assumption; that is, the excitation or ionization of the electrons only enters as a source of energy loss, but does not influence the collision dynamics. Therefore the nuclear and electronic stopping processes are taken as uncorrelated.

The energy transferred to a target atom in an elastic binary collision with an impact parameter b is given by

$$T^{\text{uncorr}} = \gamma E \sin^2(\theta/2) \quad (1)$$

where $\gamma = 4m_1m_2/(m_1+m_2)^2$; m_1 and m_2 are the projectile and target masses, respectively; E is the projectile energy in the laboratory system; and θ is the scattering angle in the centre-of-mass system.

When inelastic effects are taken into account [20], this expression is transformed into

$$T(b) = \gamma E [f \sin^2(\theta/2) + 0.25(1 - f^2)] \quad (2)$$

Table 1. Comparison of the experimental values with the calculated values for the mean projected range, the range straggling and lateral spread of 1.0 MeV Au⁺ implanted into LiB₃O₅ and SiN_{1.375}H_{0.603}. The calculated values were obtained from the TRIM98 code and the modified TRIM (MTRIM).

Target	Projected Range R_p (nm)			Range Straggling ΔR_p (nm)			Lateral Spread ΔX_p (nm)		
	Exp	TRIM98	MTRIM	Exp	TRIM98	MTRIM	Exp	TRIM98	MTRIM
LiB ₃ O ₅	279.7	219.1	272.2	54.0	33.6	45.0	34.6*	23.1	28.5
SiN _{1.375} H _{0.603}	222.3	182.3	220.4	54.6	34.6	44.4	31.5**	24.7	29.4

* Averaged value from the set of 7° and 45° as well as 7° and 60° implantation.

** Averaged value from the set of 0° and 45° as well as 0° and 60° implantation.

where $f = \{1 - Q(b)/E_{cm}\}^{1/2}$, $Q(b)$ is the energy lost by the electron excitation and E_{cm} is the energy in the centre-of-mass system. In the first order of $Q(b)/E_{cm}$, (2) is reduced to

$$T(b) = \gamma E \sin^2(\theta/2) - 2\beta Q(b) \sin^2(\theta/2) \quad (3)$$

with $\beta = m_1/(m_1 + m_2)$.

Grande *et al* [21] and Fichtner *et al* [22] suggested that the inclusion of a correlation between the nuclear and electronic processes reduces the total stopping, in particular when heavy ions interact with light targets. If such a correlation is included, the agreement between the measured and calculated values for range profile will be improved. In table 1, we also include the calculated values of the mean projected range, range straggling and lateral spread based on the modified TRIM code, which considers the correlation between the nuclear and electronic processes. It is obvious that these results show a much closer agreement with the experimental values than the original TRIM98 codes do. The maximum differences of the mean projected range, range straggling and lateral spread between the experimental and calculated values are less than 3%, 24% and 21%, respectively, for 1.0 MeV Au⁺ ions implanted into LiB₃O₅ and SiN_{1.375}H_{0.603}.

4. Conclusions

The range straggling and lateral spread of heavy ions in solids have been studied at a higher energy and for more complex targets than in previous cases. The present results show that the TRIM98 code underestimates significantly both the range straggling and the lateral spread for 1.0 MeV Au⁺ implanted into both LiB₃O₅ and SiN_{1.375}H_{0.603}. After inelastic effects are included in the nuclear stopping regime, there is a much closer agreement with experimental values than the original TRIM98 codes have.

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