SIMULATION PROPERTIES OF THIN FILMS OF INDIUM TIN OXIDE DEPOSITED ON POLYMER SUBSTRATES

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The interactions between the ion beam and matter are very complex processes that cover a large aspect of different phenomena. In this study, the energy loss, projected range, longitudinal straggling, lateral straggling and ionization of Indium Tin Oxide (ITO), Mylar and ITO/Mylar materials were simulated by SRIM code 2013. The values of energy loss, as well as the range of hydrogen ions in the samples, were obtained between 0.01 and 10Mev. The findings indicate that the growing of ITO on Mylar led to changes in the electronic and nuclear stopping powers and range in the materials. The obtained findings were compared with published data. The details of calculations are given and discussed.

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1. Introduction

Charged particles are usually categorised as light and heavy particles [1]. This work will focus on the interactions between proton and matter. The penetration of protons into materials has been a key area of interest for various purposes and in different fields for decades. The mechanism of interactions between protons and matter are classified into three groups: protons-electrons, protons-nuclei, and protons–atoms. Most protons move in a nearly straight line because their rest mass is greater than that of an electron.

However, in this work, proton interaction mechanisms parameters, such as the energy loss, projected range, longitudinal straggling, lateral straggling and ionization, are discussed.

The loss of energy by protons in materials is affected by three different incident particle energy regions [2]. The three different incident particle energy regions are classified as < 0.5MeV, > 0.5MeV and extremely high. Moreover, protons usually lose energy in matter through coulomb forces. Therefore, this study will be limited to the cases in which the incident proton's energy is from 0.01 to 10 MeV. In this region of interest, the stopping power (S) of protons is an extremely important parameter for measurements of the nuclear energy loss and atomic physics. In recent years, several works have concentrated on the calculations of energy loss, stopping power and the range of proton in matter [3]. In addition, much progress in stopping power measurements has been made for heavy ions [4]. The heavier ions and the proton theory of stopping power were reviewed and reported by many researchers [4, 5]. Conveniently, the stopping power (S) and range (R) tables are evaluated and calculated with the SRIM code [6]. The SRIM code is a Monte-Carlo calculation which follows the ion transport in the target (i.e. the stopping (S) and range (R) of ions (I) in matter (M)). The energy loss or physically equivalent parameters can be found elsewhere [4-6].

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In literature, there is little information on the interaction between protons and Indium Tin Oxide (ITO) deposited on Mylar materials [7]. Therefore, further investigations are needed to calculate the electronic and nuclear stopping powers and the range of the elements of interest. Thus, the simulation of electronic and nuclear stopping powers and the range of the elements is important not only theoretically but also in many applications.

The ITO is a well-known transparent semiconducting oxide; it is an n-type, wide-bandgap (~3.7eV) semiconductor [7]. These properties make ITO films suitable in many applications [8, 9]. However, regarding ITO thin films deposition, several studies have been performed [9]. The ITO thin films deposition on substrates has various applications. The flexible substrates may be paper, thin aluminium foil or polymer (PET, PEN, MYLAR, Transphan and polycarbonate). Among the flexible substrates, Mylar is an important commercial polymer [10, 11]. In order to deposit ITO films on Mylar substrates with certain properties and good adhesion, a detailed study on stopping power, energy loss and range properties of the films is important. In literature, the techniques used to deposit ITO thin films on substrates are the RF sputtering [12], evaporation [13], spray pyrolysis [14], ion beam deposition [15] and pulse laser deposition [16].

The purpose of this paper is to use SRIM code [15] to simulate the electronic and nuclear stopping powers and the range of ITO, Mylar and ITO/Mylar.

2. Materials and methods

2.1. The ITO Samples Preparation

ITO is an n-type semiconductor material. The structure of ITO aims to have an In_2O_3:SnO_2 ratio of 90:10wt%. The chemical composition (for an indium oxide/tin dioxide ratio of 90:10) is given as Indium: 74.52%, Oxygen: 17.60%, and Tin: 7.88% [8]. ITO films have a lattice parameter close to that of In_2O_3 and lie in the range of 10.12 to 10.31Å [9].

2.2. The Mylar samples preparation

For the purpose of this work, polyethylene terephthalate with an intrinsic viscosity of 0.60 dl/g, water content of 0.25 wt% and melting point of 250 °C was obtained from Eldritch Company. The molecular formula of Mylar is $C_{10}H_8O_4$.

2.3. ITO/Mylar samples

ITO thin films were deposited on the Mylar substrate. The density of ITO was 7.14 g/m^3 at 293°K. The density of Mylar was 1.38g/cm^3 at 293°K.

3. Theoretical details

A number of codes dealing with the transport of hydrogen ions within compound materials exist. SRIM code [10] is one of them, and it runs on Linux, Mac OS and windows. The energy deposition phenomena is usually described by the stopping power (-dE/dx). The total stopping power (S_{Total} or S_T) is given as the sum of electronic (Se), nuclear (Sn) and reaction energy transfer mechanisms. S_{Total} or S_T is given by the following:

$$S_T = -\frac{dE}{dx} = S_n + S_e + S_{reaction} \tag{1}$$

3.1. Electronic Energy Loss

The electronic energy loss (Se) of a highly energetic ion in a solid is stated as follows [11]:

$$S_e = \left(-\frac{dE}{dx}\right)_e = \frac{4e^4 Z_P^2\ Z_t N_t}{mev^2}\left[ln\left(\frac{2m_e v^2}{I}\right) - ln\left(1-\frac{v^2}{c^2}\right) - \frac{v^2}{c^2}\right] \tag{2}$$

Where v and Z_pe are the velocity and charge of the projectile ions respectively; Z_t and N_t are the atomic number and number density of the target atoms respectively; e is the electron elementary charge; and m_e is the electron rest mass. The parameter I is the target excitation or ionization.

3.2. Nuclear Energy Loss

The nuclear energy loss (Sn) is obtained from the following expression [11, 12]:

$$S_n = \left(-\frac{dE}{dx}\right)_n = N\frac{\pi^2}{2}Z_1 Z_2 e^2 \alpha \frac{M_1}{M_1+M_2} \quad (3)$$

Where Z_1e is the projectile nuclear charge; Z_2e is the target nuclear charge; *I* is the target average excitation; and N is the Avogadro number.

3.3. The Range of ions

The range of ions in a material can be obtained from the loss of energy of a charged particle. After a charged particle penetrates a material of thickness x, the energy loss can be computed by the range (R) of the ion in the material. The range of ions in elements is given by the following:

$$\mathrm{R} = \int_0^{\mathrm{E_0}} \left(-\frac{\mathrm{dE}}{\mathrm{dx}}\right) \mathrm{dE} \quad (4)$$

Where, dE/dx is the energy loss of both the electronic and nuclear parts of an ion with energy E. Due to the importance of ITO and PET materials in advanced device and nuclear applications, better Se and Sn parameters for possible improvement are needed.

3.4. Computational methods

The SRIM-2013 computer code was used to estimate the electronic and nuclear stopping powers and the range of ion beams in ITO, Mylar and ITO/Mylar with energy of 0.01 to 10.0MeV. Simulations were performed using detailed calculations with full damage cascades' analysis for samples. Collision cascade damage was taken into consideration in the analysis using 99000 ions on the spot. Tables 1 to 4 give the description of ions and targets used in the SRIM analysis of ITO, Mylar and ITO/Mylar. For ITO composite, SRIM inputs, Indium (In), Tin (Sn) and Oxygen (O), were added in percentage compositions.

Table 1. Hydrogen ion description used in SRIM calculations.

Element	Atomic Number	Mass (a.m.u)	Ion Energy Range (keV)	
			Lowest	Highest
Hydrogen	1	1.008	10	10000

Table 2. ITO elemental composition used in SRIM calculations, density, ρ =7.14 g/m^3.

Element	Atomic Number	Weight (a.m.u)	Stoich.	Atom%
Oxygen, O Indium, In	8 49	15.999 114.82	3 2	33.33 22.22
Tin, Sn	50	118.71	1	11.11
Oxygen, O	8	15.999	3	33.33

Table 3. Mylar elemental composition used in SRIM calculations, density, ρ =1.38g/cm^3.

Element	Atomic Number	Weight (a.m.u)	Stoich	Atom%
H C	1 6	1.008 12.011	8 10	36.36 45.45
O	8	15.999	4	18.18

Table 4. ITO/Mylar Films elemental composition used in SRIM calculations, density, ρ =1.38g/cm^3.

Element	Atomic Number	Weight (a.m.u)	Stoich	Atom%
O In	8 49	15.999 114.82	3 2	9.68 6.45
Sn	50	118.71	1	3.23
O	8	15.999	3	9.68
H	1	1.008	8	25.81
C	6	12.011	10	32.26
O	8	15.999	4	12.90

4. Results and discussion

4.1. The Results of Electronic and Nuclear Energy Loss of Ions in ITO

Table 5 gives the ion range (R), longitudinal range (LR), lateral straggling (LS), and electronic and nuclear stopping powers in ITO, Mylar and ITO + Mylar composite for 10 MeV H^+-ions. The electronic stopping powers (S_e) of ITO are given at 0.02447 to 0.1120MeV/gmcm^2, while the nuclear stopping powers (S_n) of ITO are given at 0.00001186 to 0.001896MeV/gmcm^2. The ion projected range, longitudinal range and lateral straggling of ITO are given at 127.1 to 552310.0 nm, 89.5 to 29940.0 nm and 73.7 to 45690.0 nm respectively. Fig. 1 shows the electronic and nuclear stopping powers dependence on ion energy.

Table 5. Ion range, straggling, and stopping powers in ITO, Mylar and ITO/Mylar for 10 Me Hydrogen ions.

Parameter	**ITO**	**Mylar**	**ITO/ Mylar**
Ion Range (nm)	552310	930640	722130
Longitudinal Straggling (nm)	29940	41690	38060
Lateral Straggling (nm)	45690	26020	55740
Stopping power-electronic (MeV/ gmcm^2)	0.02447	0.04311	0.02602
Stopping power-nuclear (MeV/ gmcm^2)	0.00001186	0.00002248	0.00001274

Fig. 1 clearly indicates that most of the ion energy is lost to electronic events (ionization), and very little to nuclear events that produce atomic displacements/vacancy defects. The nuclear stopping power increases at low ion energies; thus, one may expect that most of the vacancies are produced at the end region of the ion range. The electronic stopping power is thousands of times greater than the nuclear stopping power at 10 MeV. Thus, most of the energy dissipation of the ion is due to electron energy transfers, which lead to cleavage of polymer chains and local melting of material within the hotspots around the primary ion trajectory.

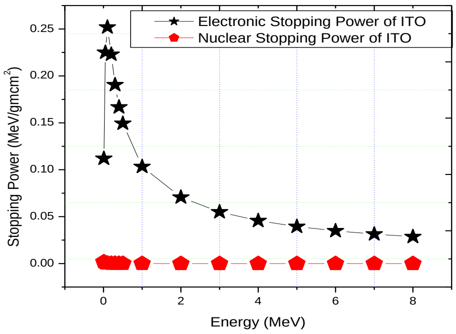

Fig. 1. Shows electronic and nuclear stopping power of hydrogen ions in ITO at density of 4.36g/cm^3.

4.2. The Results of the Range (nm) of Hydrogen Ions in ITO Target

Fig. 2 gives the range-energy relationship for protons in ITO from 0.01 to 10 MeV.

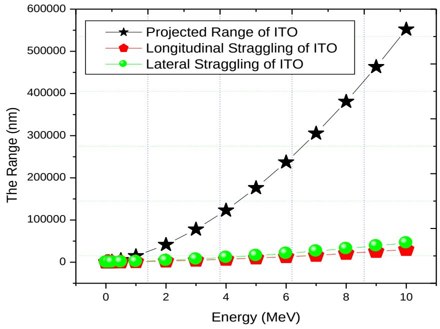

Fig. 2. Shows the range of hydrogen ions in ITO at density of 4.36g/cm^3.

4.3. The Results of Electronic and Nuclear Energy Losses of Ions in Mylar Substrates

The electronic stopping powers (S_e) of Mylar are given at 0.04311 to 0.4108 MeV, while the nuclear stopping powers (S_n) of Mylar are given at 0.00002248 to 0.006983 MeV. The ion projected range, longitudinal range and lateral straggling of Mylar are given at 197.4 to 930640.0 nm, 52.8 to 41690.0 nm and 54.7 to 26020.0 nm respectively.

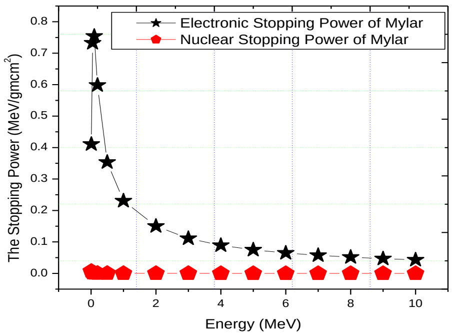

Fig. 3. Shows electronic and nuclear stopping power of hydrogen ions in Mylar at density of 1.397g/cm^3.

4.4. The Range of Hydrogen Ions in Mylar Substrates

Fig. 4 gives the range-energy relationship for protons in Mylar from 0.01 to 10 MeV.

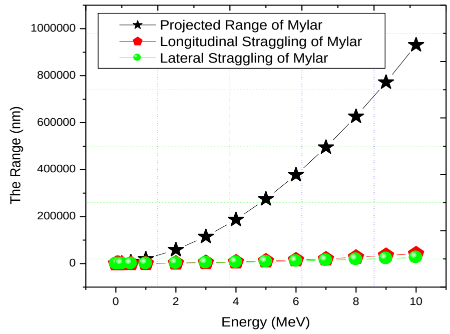

Fig. 4. Range (nm) nm of hydrogen ions in Mylar at density of 1.397g/cm³.

4.5. The Results of Electronic and Nuclear Energy Losses of Ions in ITO/Mylar

The electronic stopping powers (S_e) of ITO/Mylar are given at 0.02602 to 0.1324 MeV, while the nuclear stopping powers (S_n) of ITO/Mylar are given at 0.00001274 to 0.002318 MeV. The ion projected range, longitudinal range and lateral straggling of ITO/Mylar are given at 165.9 to 722130.0 nm, 105.2 to 38060.0 nm and 88.3 to 55740.0 nm respectively.

Fig. 5 shows the comparison of the stopping powers between ITO and ITO/Mylar composite at an energy range close to 10 MeV.

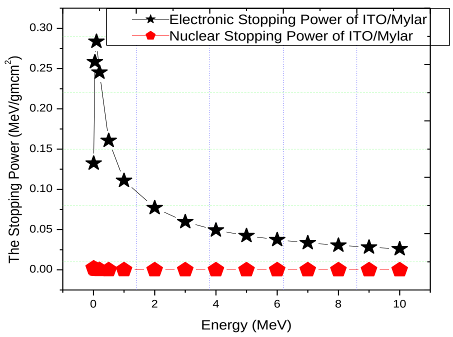

Fig. 5. Shows electronic and nuclear stopping power of hydrogen ions in ITO/Mylar at density of 03.11620g/cm³.

4.6. The Range of Ions in ITO/Mylar

For practical purposes, the (normal) projected range, R_p, is mostly of interest, since it characterizes the implantation depth with respect to the surface. For more precise data of projected range, transport theory calculations have to be performed. Alternatively, computer simulation, the SRIM computer code, can be employed. Fig. 6 is a plot of projected range vs. incident ion energies for implantation of H ions into amorphous ITO/Mylar. Fig. 6 shows the range of hydrogen ions in ITO/Mylar for a broad energy range. Also, Fig. 6 gives the range-energy relationship for protons in ITO/Mylar from 0.01 to 10 MeV.

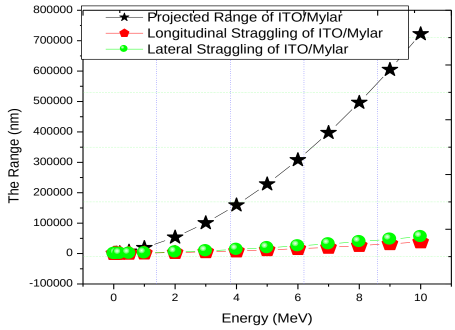

Fig. 6. The range (nm) of hydrogen ions in ITO/Mylar at density of 03.11620g/cm³.

5. Conclusions

In conclusion, the stopping power and range of protons in ITO, PET and ITO deposited on PET are calculated by SRIM code. It was found that the properties of ITO/PET depend strongly on the film thickness. The investigation of the lateral range and lateral straggling are important to determine detailed trajectories of ion beams in matter. Since there are limited experimental measurements of lateral straggling, it is necessary to find accurate data for numerical simulations. The present results of the energy loss and range for these materials at energy of 0.01 to 10 MeV might be useful in studies on the effects of various ions on these materials.

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References

[1] J. E. Turner, *Atoms*, Radiation, and Radiation Protection, 2nd Edn., Wiley, New York, 1995.
[2] M. Nastasi, J. W. Mayer, J. K Hirvonen, Ion-Solid Interactions: Fundamentals and Applications, Cambridge Solid State Science Series, Cambridge University Press, 1996.
[3] M. O. El- Ghossain, Int. J. Phys. **5**(3), 92 (2017).
[4] J. F. Ziegler, J. P. Biersack, U. Littmark, The stopping and range of ions in solids, Pergamon, New York, 1985.
[5] J. F. Ziegler, J. Appl. Phys. **85**, 1249 (1999).
[6] E. Rauhala, N. P. Barradas, Fazinic, S. M. Mayer, E. Szilágyi, M. Thompson, Nucl. Instr. Meth. B **244**, 436 (2006).
[7] H. J. Möller, Prog. Mater. Sci. **35**, 205 (1991).
[8] M. K. M. Ali, K. Ibrahim, O. S. Hamad, M. H. Eisa, M. G. Faraj, F. Azhari, Rom. J. Phys. **56**, 730 (2011).
[9] S. A. Knickerbocker, A. K. Kulkarni, J. Vac. Sci. Technol. A **13**(3), 1048 (1995).
[10] L. Hao, X. Diao, H. Xu, B. Gu, T. Wang, Appl. Surf. Sci. **254**, 3504 (2008).
[11] O. Tuna, Y. Selamet, G. Aygun, L. Ozyuzer, J. Phys. D: Appl. Phys., 43 (2010).
[12] S. Naseem, I.A. Rauf, K. Hussain, N. A. Malik, Thin Solid Films **156**, 161 (1988).
[13] D. J. Seo, S. H. Park, Physica. B **357,** 420 (2005).
[14] C. Liu, T. Mihara, T. Matsutani, T. Asanuma, M. Kiuchi, Solid State Commun. **126**, 509 (2003).
[15] D. Ginley, B. Roy, A. Ode et al., Thin Solid Films **445**, 193 (2003).
[16] J. F. Ziegler, M. D. Ziegler, J. P. Biersack, Nucl. Inst. Meth. Phys. Res. B **268**, 1818 (2010).