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Estimation of Displacement per Atom (dpa), Range and Energy Loss during Irradiation of Low Energy ions (150keV) of He, Ne, Ar and Xe on Bismuth Telluride Target using SRIM Simulations

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Abstract— ***This paper present the simulation study of irradiation of 150 keV energy ions of He, Ne, Ar and Xe on Bismuth Telluride(Bi_2Te_3) as target material. The simulation software SRIM and TRIM -2013 is used for this study. For this study, we simulated 5000 ions of energy 150 keV on Bismuth Telluride monolayer target. Bismuth Telluride is one of most important thermoelectric (TE) material and extensively used in TE based devices. In this study, ion range, lateral range distribution, ionization and energy loss were simulated and graphically presented. Using vacancy created by ions, displacement per atom (dpa) is estimated. The result shows as the ion becomes heavier, the percentage of energy loss through ionization decreases and to recoil gradually increases. The incident energy (150keV) loss for He ions was maximum of about 95.93% whereas for Xe ion it was least around 8.23% due to ionization process. The mean projected range was found to be maximum for He ion of 589.2 ± 189.7 nm and minimum for Xe ions 44.8 ± 24.1 nm. The skewness was found to be positive for all ions except for He ions which was found to be negative. The dpa was calculated for different fluences and for He, Ne, Ar and Xe, it is found to be 0.04, 11.72, 29.94209 and 161.66 respectively for the dose 1×10^{16} ions/cm^2.***

Index Terms— ***Displacement per atom, Irradiation, Ionization, Range***

I. INTRODUCTION

Ion beam irradiation effects on the thermoelectric materials is an emerging field of study. The higher damaging efficiency of energetic ions in much shorter time can be crucial in thermoelectric materials to enhance the thermoelectric power factor. The effect of ion beam irradiation of 350 eV of He, Ar, and Xe on PbTe thin films synthesized using thermal evaporation technique has been reported [1-2].Similar results were also obtained by implanting N ions in $SrTiO_3$ thin films [3].

In Ion beam irradiation process, the energetic ions beam passes through target materials and loses energy until it come to rest through large number of cascading collisions with nuclei and electrons of target material. When ion comes to rest in target material it is called ion implantation. The ions lose their energy to the target material mainly through two processes namely electronic and nuclear interactions. These processes are almost independent of each other.

In nuclear interactions, the fast moving ions collide with atomic nuclei of the target material and lose its energy through nuclear collisions. This process is known as nuclear energy loss. This interaction is elastic in nature. The energy transferred through nuclear interactions contributes to atomic displacements, lattice vibrations and other structural modifications. In electronic interaction, the transfer of kinetic energy of the ions to the electrons in target material. This process is called as electronic energy loss. It is defined as the rate at which ions lose energy to the electrons as they passes through the material. This transferred energy can induce electronic excitations, ionizations, and the generation of electron cascades in the material. At low energies nuclear interaction dominates and it decreases with energy increase and at high energy electronic interaction dominates[8].

In ion-solid interactions, the rate at which an energetic ion loses energy per unit distance travelled through the material is called stopping power or linear energy transfer(LET). The stopping power of an ion in a target represents the energy loss (dE)of the ion in the target per unit length(dx). It is defined by the following relationship: [4]

$$\text{LET} = -1/\rho \ . \ dE/dx$$

The LET consist of two processes viz the electronic LET and the nuclear LET.

$$\text{LET}=\text{LET}_{\text{electron}} + \text{LET}_{\text{nuclie}}$$

The Bethe-Bloch formula is commonly used to calculate *electronic energy loss*. *Nuclear stopping power* is estimated using the binary collision approximation(BCA). Electronic Stopping Power describes the energy loss per unit path length of an ion due to *interactions with the electrons* in the target material. The Bethe-Bloch formula is commonly employed to calculate the electronic stopping power. [5]

$$-\left(\frac{dE}{dx}\right)_{elec} = K.\frac{Z_1^2 Z_2^2}{A_2 \beta^2}.\left[\ln\left(\frac{2m_e\beta^2\gamma^2T_{max}}{I^2}\right) - 2\beta^2\right.$$

Here, K = constant, Z_1 and Z_2=charges of incident ion and target atom, A_2=atomic mass of target atom, β =ion velocity normalized to speed of light, γ =relativistic factor,

m_e=electron mass,T_{max}=maximum energy transfer allowed in a single collision, I= average ionization potential of the target material.

Nuclear Stopping Power describes the energy loss per unit path length of an ion due to *interactions with atomic nuclei* in the target material. The binary collision approximation (BCA) provides useful model to estimate the nuclear stopping power [5-7]

$$-\left(\frac{dE}{dx}\right)_{nuc} = n.\pi.\left(\frac{d^2}{2}\right).[\left(Z_1\frac{Z_2}{M_1}\right)^2.\frac{2m_1E}{\hbar^2v^2}]$$

Here, n= no. density of target atoms, d=interatomic spacing, Z_1 and Z_2= charges of incident

Ion and target atom, M_1=mass of incident ion, m_1=reduced mass of ion-target system, E=K.E. of incident ion, $\hbar$ =reduced planck constant, v=velocity of incident ion.

II. RANGE

The range of ions in a material is the total distance travelled before losing all its energy and coming to rest. The discrete nature of energy loss processes causes uncertainty in energy and it is called energy straggling. The ions travels a zigzag path in target material. The implantation doses are generally higher (~ 10^{12} ions/cm ^{2}) so, ion trajectories can be estimated using statistical methods. The deviation in range due to energy straggling is called range straggling [7-9]. So, the total range is the sum of all different paths that an ion travels in target material.

The projected range is the average depth from the surface to where the ion comes to rest measured in direction parallel to incident direction. The light ion will transfer small energy during collisions and so the range will be comparatively large. Due to which damage is spread over large volume of the material. The heavier ion will have shorter range and damage is confined to smaller volume. The energy from light ion is transfer to lattice by electronic interaction whereas for heavy ion it is by nuclear interaction [9, 13].

III. METHODOLOGY

We have used a software developed by Ziegler and Biersack in 1985 called SRIM (stopping and range of ion in matter) which calculates stoppage and range of ions with energy 10 eV to 2 GeV [9, 14, 16]. . It is a group of computer programs that calculates interaction of ions with matter according to Monte-Carlo simulation. In this work SRIM-2013 has been used. The SRIM tables of stopping power, projected range and linear energy transfer(LET) verses ion energy were used for visualization and statistical presentation. For estimation of ion range, damage , collision events etc TRIM (Transport of ion in matter) is used. This program has good accuracy with 5-10% error [9]. This program uses some approximations like Binary collision, recombination of knocked off atoms with the vacancies is neglected etc for simulation[8-9].

Choice of the Target

Bismuth Telluride (Bi_2Te_3)[10,11] has been identified as one of most important thermoelectric material as it has highest thermoelectric power of around 1 at room temperature. Bi_2Te_3 is a semiconductor with bang gap of around 0.12 eV. Bi_2Te_3 based TE materials are extensively used in TE devices. Keeping these properties in mind we choose Bismuth Telluride as target material for the study.

A study of implantation of antimony and boron ion on silicon target was done and shown that lighter ion causes more ionization as compared to heavy ions [13]. The range and penetration profile of Ar, Kr Xe and U on silicon target was studied and found that loss of nuclear energy decrease with incident ion energy [15].

IV. RESULTS AND DISCUSSION

The figure 1 shows the range (distance) profile as a function of the energy of Ar, He, Xe and Ne ions as obtained by SRIM-2013 The distance travelled by ions in material increases with energy. At same initial energy the distance travelled by ions in target material decreases with increase in atomic number. It is found that at 150 keV energy, lighter He ion has travelled a distance of 590 nm where as Xe has travelled a distance of 41.1 nm in Bi_2Te_3.

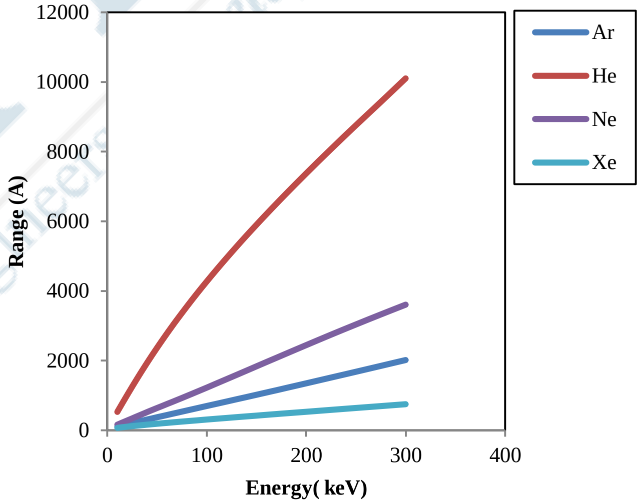

Figure 1: The range vs ion energy profile of Ar, He, Xe and Ne ions.

The figure 2 shows the profile of electronic and nuclear energy loss with irradiation energy for He, Ne, Ar and Xe ions. The electronic energy loss increase with increase in ion energy. For energy of 150keV, the Ar has loss of 34.23 eV/ Å where as He has 26 eV/ Å. In case nuclear energy loss, Xe has 249 eV/ Å and He has 0.24 eV/ Å.

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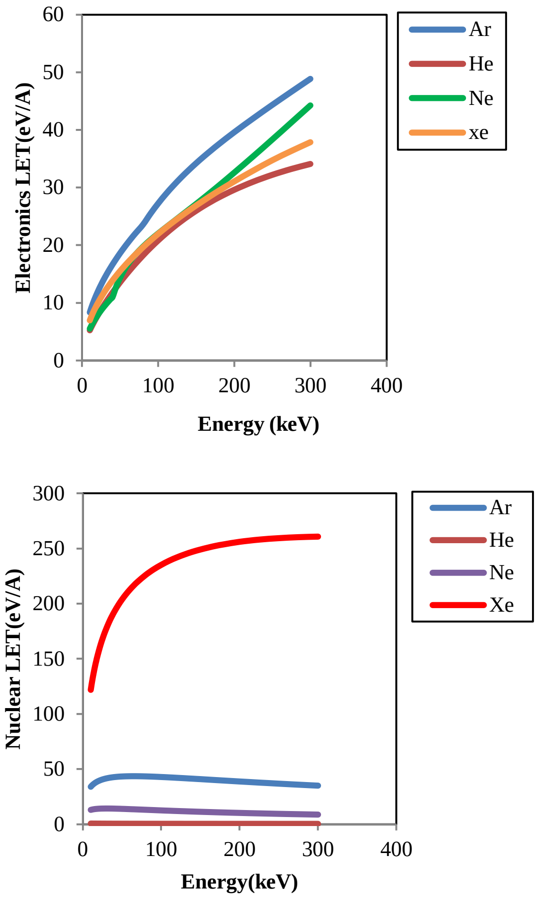
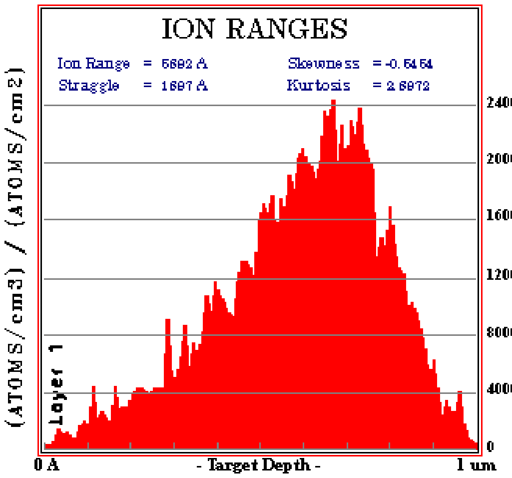


Figure 2 : Profile of Electronic (top) and Nuclear energy loss (bottom) with irradiation energy for He, Ne, Ar and Xe ions



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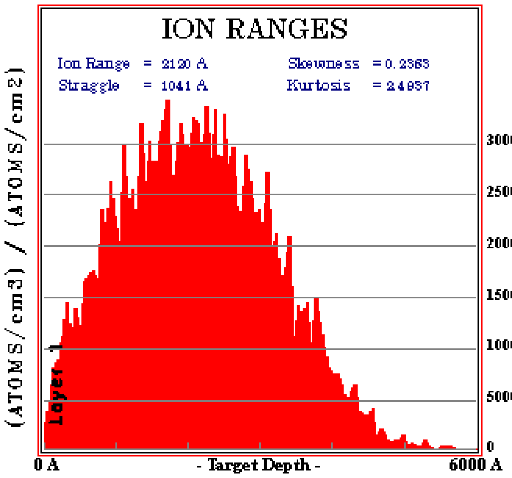

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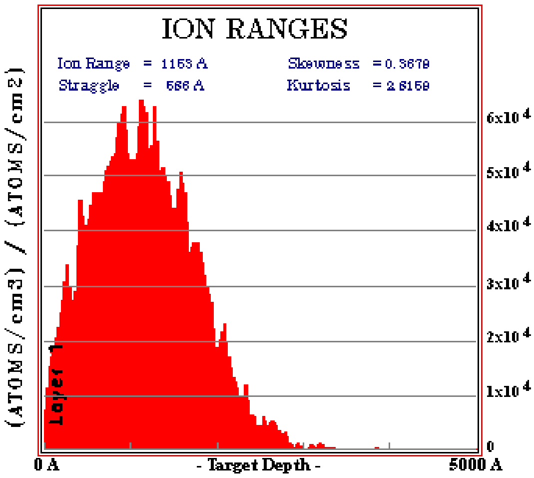

(c)

Ion Ranges

The figure 3(a-d) shows the profile of ion range with doping of Argon, Helium, Xenon and Neon ion on Bi-Te alloy target with the energy of 200 keV . The details of ion range, straggle, skewness and kurtosis is shown in the table 1. It is found that with simulation, the distance travelled in target material decreases with heavier atoms. The He ion has the maximum range and straggle of 589.2 ± 212 nm and least for Xe with 44.8 ± 24.1nm. The skewness for He ion is negative , which means the left tail of the distribution is longer than the right (figure 3(a)). The skewness for other three ions is positive which implies graph is skewed towards right (figure 3(c-d)).. The kurtosis is positive for all plots which indicates that the distribution has heavier tails than the normal distribution.

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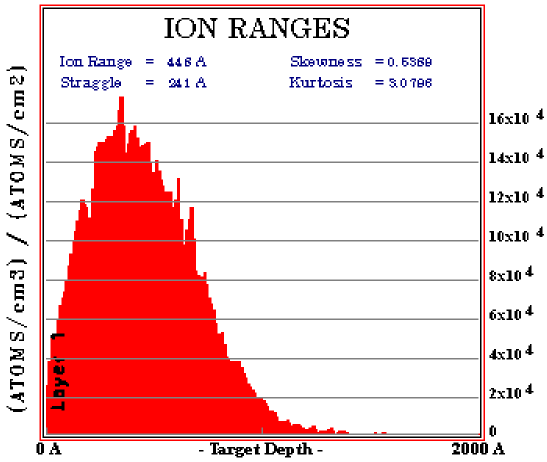


(d)

Figure 3(a-d): The plots showing ion range profile for He, Ne, Ar and Xe ions in Bi-Te target material

Table 1: Average range value for He, Ne , Ar and Xe ion in Be-Te target

Parameter	Helium	Neon	Argon	Xenon
Ion Range(	5892	2120	1153	448
Straggle	1897	1041	586	241
Skewness	-0.5454	0.2383	0.3679	0.5389
Kurtosis	2.8972	2.4937	2.8159	3.0796

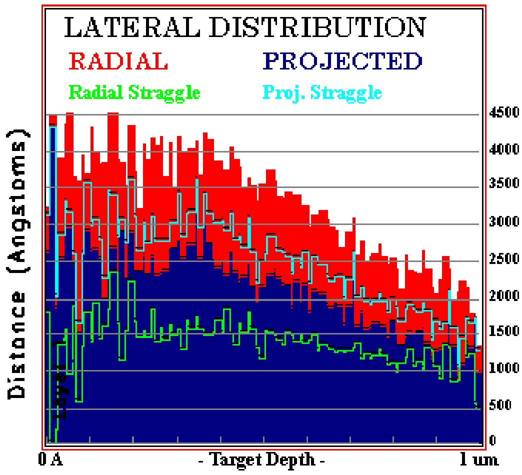
Lateral Range Distribution.

The figure 4(a-d) shows the profile of lateral range distribution of ions within the target material. For He ion, the lateral and radial range as well as straggle is high at the surface and decreases slowly with target depth, whereas for Ne and Ar, it is more or less the same and for Xe it is low at the surface and increase gradually with the target depth (figure 4 (a-d)).

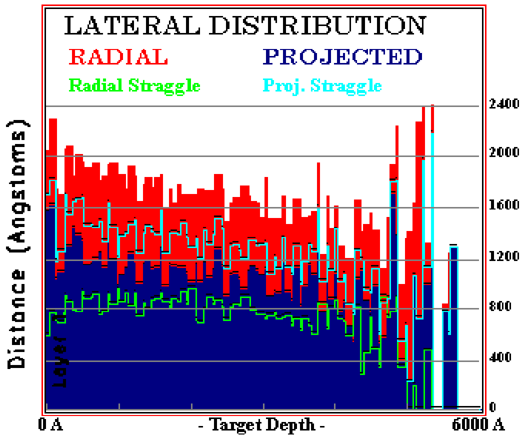
The lateral projected range helps in understanding of horizontal spread of ion in material and radial range in distribution of ions in the perpendicular direction. The table 2 show the values of lateral and radial range with straggle for the ions used for this study. It show that the path travelled in target material is more for lighter ions for example for He, lateral range is 589.2 ± 189.7nm and radial is 312.4 ± 149.2 nm than those of heavier ones .

Table 2: Lateral range distribution for He, Ar, Xe and Ne ions in Bi-Te target

	He (Å)	Ne (Å)	Ar (Å)	Xe (Å)
Longitudinal	5892 ± 1897	2120 ± 1041	1153 ± 586	448 ± 241
Lateral Projection	1985 ± 2450	1083 ± 1342	563 ± 701	165 ± 214
Radial	3124 ± 1492	1701 ± 833	876 ± 453	262 ± 159



(a)



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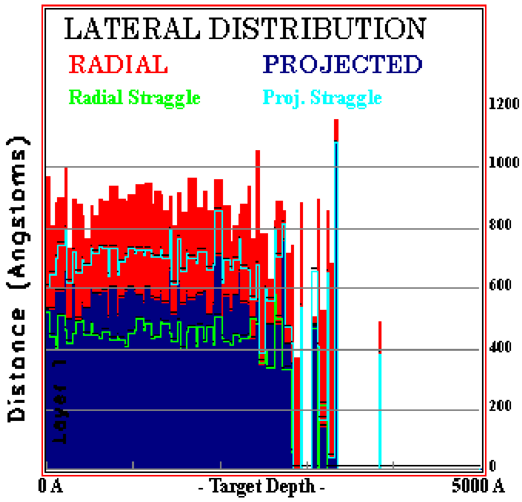

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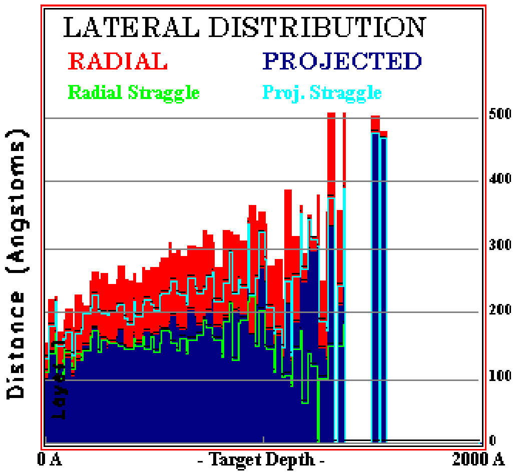
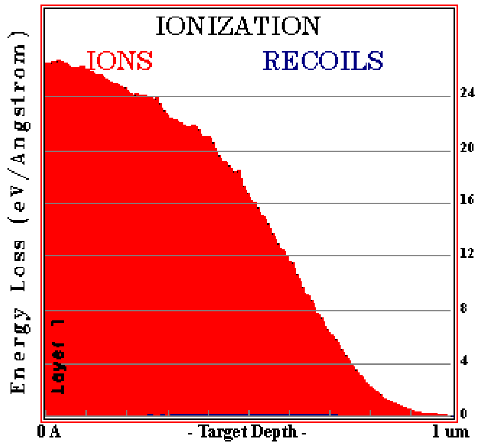


(d)

Figure 4 (a-d) : The plots showing lateral range distribution profile for He, Ne, Ar and Xe ions in Bi –Te target material.

Ionization

The result of ionization of Bi2Te3 atoms by incident ions are shown in the figure 5(a-d). It is plot of the energy loss vs penetration depth for ionization of target material. The calculation shows 95.93% of incident energy (150keV) of He ion is lost during ionization and 0.43 % only through recoils figure 5 (a). In case of Ne and Ar ions the 55.11% and 34.81 % of total energy loss is lost through ionization process whereas with recoil the energy loss is 7.50 % and 12.32% respectively (figure 5(c-d)). For 150 keV Xe ion 8.23 % of energy is lost to ionization and with recoil it is 19.79 % (figure 5 (d). It is clear from the results, that as the ion becomes heavier, the percentage of energy loss decreases through ionization while it increases with recoil.



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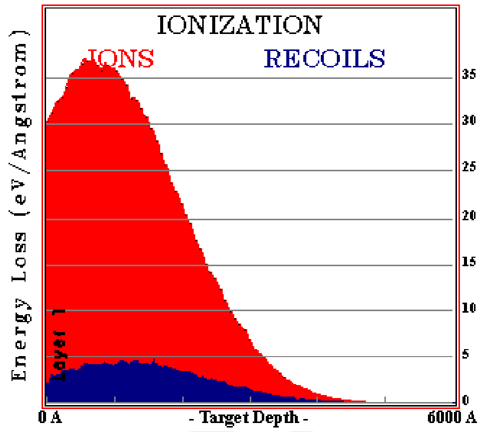

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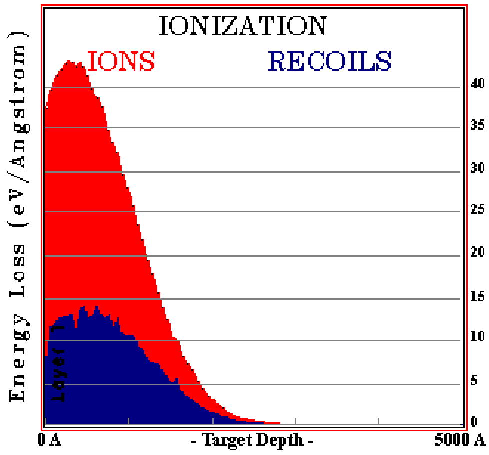

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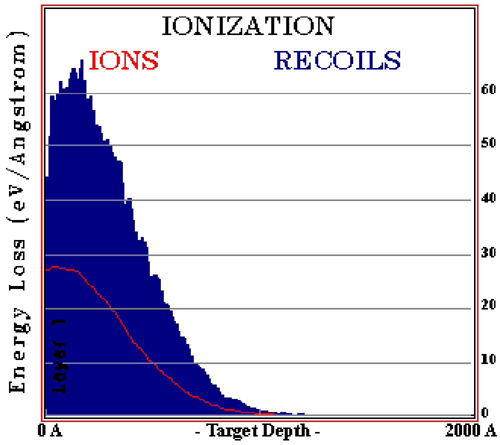

(d)

Figure 5 (a-d) : The plots showing the energy loss vs target depth with ionization process for He, Ne,Ar and Xe ions.

Collision events

The results of the collision events of Ar, He, Xe, Ne ions shown in the figure 6(a-d).The curve shows the target displacements, vacancy and recoils created by ions in the target material. The vacancies calculated here are obtained from output file of vacancy.txt file of TRIM program. The table 3 summarizes the total vacancies created by calculating area under the curve. The total vacancies here are the sum of

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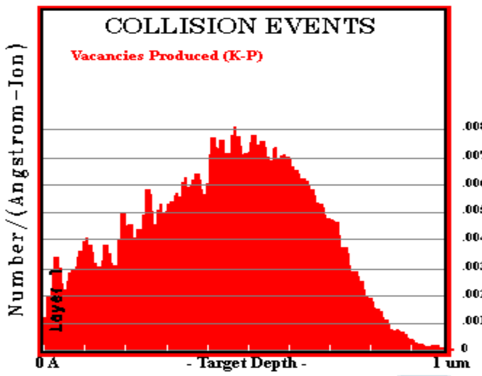
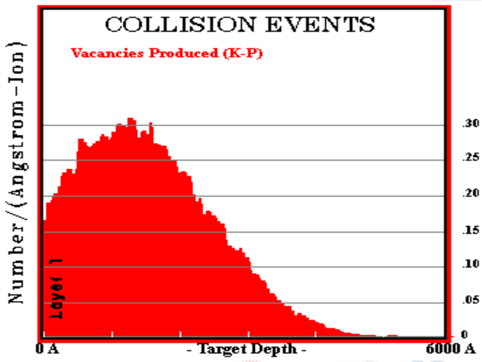
vacancies created by ions and recoils. The vacancies created by He and Xe ion is 0.012123 and 4.6623 respectively. The total vacancies are used in estimation of displacement per atom(DPA) in the target material by using the equation shown below .

$$DPA = \left(\frac{vacancies}{ions \times Å}\right) \times \frac{10^8(\frac{Å}{cm}) \times Fluence(\frac{ions}{cm^2})}{\text{density } (\frac{atoms}{cm^3})}$$

The DPA value is a measure of the damage caused by the displacement of atoms from their original lattice positions due to high-energy collisions . We have used different fluences i.e dose(ions/cm^2)for estimation of dpa. The density of the target material estimated by TRIM is 2.884×10^{22} atoms/cm^2, which is used for this calculation. The calculation for dpa for different fluences is shown in table 4.



(a)



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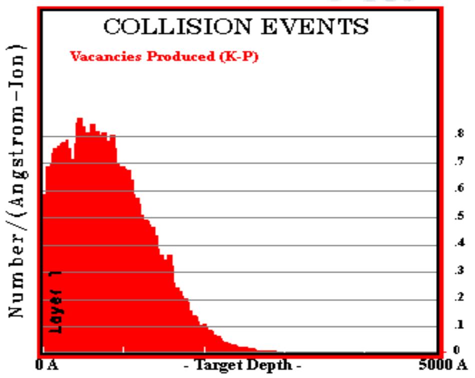

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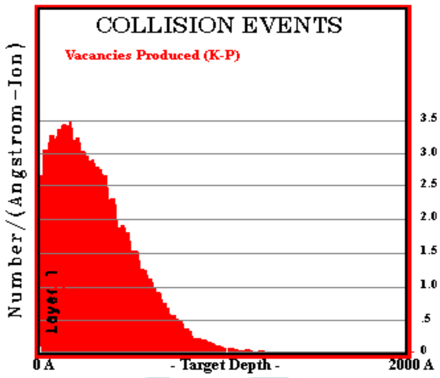

(d)

Figure 6(a-d): The plots showing the vacancy distribution for He, Ne,Ar and Xe ions

Table 3: Vacancy created during ion implantation

Ion	Vacancies by Ions	Vacancies by Recoil	Total (Vacancy)
Helium	0.007392	0.004731	0.012123
Neon	0.03564	0.3025	0.33814
Argon	0.05243	0.8111	0.86353
Xenon	0.1123	4.550	4.6623

Table 4: Details of ion implantation in Bi-Te target

Ion	Mean projected range ± straggling (nm)	Ion fluences (ions/cm^2)	Peak damage (dpa)
150 keV He$^+$	589.2 ± 189.7	5×10^{14}	0.021018
		1×10^{15}	0.042035
		5×10^{15}	0.21018
		1×10^{16}	0.42035
150 keV Ne$^+$	212.0 ± 104.1	5×10^{14}	0.586234
		1×10^{15}	1.172469
		5×10^{15}	5.86234
		1×10^{16}	11.72469
150 keV Ar$^+$	115.3 ± 58.6	5×10^{14}	1.497105
		1×10^{15}	2.994209
		5×10^{15}	14.97105
		1×10^{16}	29.94209
150 keV Xe$^+$	44.8 ± 24.1	5×10^{14}	8.083044
		1×10^{15}	16.16609
		5×10^{15}	80.83044
		1×10^{16}	161.6609

Conclusions

The TRIM-2013 simulation of ion irradiation (implantation) of inert gas ions on Bismuth Telluride (Bi_2Te_3) target shows that as the ion becomes heavier, the percentage of energy loss through ionization decreases while contribution of recoil gradually increases. The simulation result indicate that for a 150 keV He ions, 95.93% of incident energy is lost through ionization, while only 0.43 % is lost through recoils. On the other hand, for the same incident energy for Xe ions 8.23 % of the energy is lost to ionization and with recoil it is 19.79 %. Additionally, the simulation, reveals that the distance travelled in target material decreases as the atomic mass of the ion increases. The Mean projected range was maximum for He ion of 589.2 ± 189.7 nm and minimum for Xe ions 44.8 ± 24.1 nm. The skewness was found to be positive for all ions except for He ions which was found to be negative. The vacancies created by 150 keV He ion was least 0.012123 and Xe ion produced maximum vacancies of 4.6623 respectively. The peak damage (displacement per atom) increases with fluence and was maximum for Xe ions for fluence 1×10^{16} ions/cm^2.

In future, we intend to carryout carry out experiment of irradiation of low energy inert gas ions on Bismuth Telluride (Bi2Te3) and lead telluride. These results of irradiation parameters will supplement and help us understanding of ion-matter interaction and shall be used for the study of the thermoelectric properties.

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