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CALCULATION OF THE RATE OF HELIUM ION DISPERSION IN GALLIUM ARSENIDE COMPOUND

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Abstract. Nuclear dispersion is an important aspect in the process of slowing down ions by transferring their momentum to the target atoms and in determining path of the ion. This paper concerns the quantitative evaluation of the mechanism at which helium ions lose their energy when penetrate into a solid and the eventual distribution of the helium ion while stopping inside the Gallium Arsenide compound (GaAs). The first order effects of the atoms of the compound such as the electronic excitation of the atom, the lattice damage incurred to it, as well as the production of phonons in Gallium Arsenide due to the helium ions are also taken into account. The main finding is the mechanism of penetration of helium ions in GaAs, which is affected by the energy, the angle of incidence, and penetration density of the helium ions. It is found out that the energy has major impact than the angle of incidence in the interaction.

Introduction

The rate of energy loss when particles penetrate or move through a material is an important aspect in modern microelectronics industry. The implantation of ions is applicable in a broad spectrum at this moment of time. The calculation of energy loss of ions in materials or samples should be accurate so as to advance further in technology as well as to gain knowledge in various other branches of science. The stopping power of ions, penetrating into a material is affected by the dispersion process such as [1]:

- I. The excitation and ionization of target electrons
- II. Electron capture
- III. The excitation and ionization of ions
- IV. Displacement of the nucleus

Normally, the method used to calculate the penetration depth in a medium is based on the theory of binary collision approximation (BCA) [2]. This method implies that the movement of ions in a sample is considered as a successful collision between the incident ions with the atoms in the sample. Furthermore, the classic integral dispersion is for each collision is solved using numerical integration. A good and viable program used to simulate the movement of ions in a sample or BCA is TRIM (Transport of Ions In Matter) or now called SRIM (Stopping and Range of Ions in Matter) which is based on the ZBL electronic stopping and inter-atomic potential [3, 4].

During the penetration of the ion, high-energy ions will naturally be attracted to the target atom and will consequently collide with the nucleus and electrons of the atom. This interaction will cause the loss of energy of the incident ion which is called stopping power of an ion. At energy ranging from 0 to 10 keV/amu, the stopping power is divided into two types, which are nuclear stopping and electronic stopping. The slowing down force for this stopping power can be given as [5]:

$$S = \left(\frac{dE}{dx} \right) = \left(\frac{dE}{dx} \right)_{\text{nuclear}} + \left(\frac{dE}{dx} \right)_{\text{electronic}} \quad (1)$$

It is well known that the nuclear stopping is the elastic collision that happens between an ion and a target atom [6]. If the repulsive potential energy between the two atoms is known, the value of the nuclear stopping can be calculated. The nuclear stopping increases when the mass of the ion increases. As the movement of light ions gets slower in a heavy material, the nuclear stopping gets weaker than the electronic stopping at certain energies. For high energy ions, the process of slowing ions at first is due to the nuclear stopping and the ion tends to move close to a straight trajectory (nuclear collisions that happen between light ions like H and He sometimes are so strong that they cause the movement of ions to become more random) [7]. Ion collisions with the nucleus of the atom become more frequent when the movement of the ion is slow or close to stopping. The target atom is removed from its lattice when the atom is subjected to sufficient recoil energy and would in turn create a stream from the next collisions in the lattice. This collision stream is the main reason behind the damage to lattice during the implantation of the ion [1].

Experimental Details

The simulation SRIM (Stopping and Range of Ions in Matter) is used in this paper to predict these phenomena together with TRIM (Transport of Ions in Matter) Calculation of Full Damage Cascade. This simulation can show the full animation of the penetrating process, the recoil cascades and also the mixing of target atoms [6]. In order to make precise evaluations of the physics of every single encounter between the ion and target atom, the calculation is triggered for one ion at a time. The calculation runs even it is interrupted awhile and the output results can be saved and used later. The calculation period is varied for different ion, which may range from a second to a few minutes for each ion. The results obtained acquired averaging over many simulated particle trajectories [7].

The target atoms utilized in the simulation, GaAs has a band gap energy of $E_g = 1.42$ eV at room temperature with a density of 5.316 g/cm³. In this paper, the damage induced by helium ion on the GaAs layer depth = 100 nm, 400 nm and 1000 nm is simulated. The energies for the incident ions are varying from 100 keV up to 1 MeV, and the angles of incidence of the ions are varying from 0° to 60°.

GaAs compound is being discussed as it is ideally suitable for the development of high speed microwave circuits and also enabling transistors made from them to function at frequencies in excess of 250 GHz. Besides, GaAs has a wide direct band gap material. Therefore, it can be used to emit light efficiently and makes them an excellent material for space and optical windows in high power application [8, 9]. By the simulation of detailed calculation with full damage cascades, the plots of ion trajectories, depth vs. Y-Axis, depth vs. Z-Axis, transverse view, ionization, phonons, collision events, atom distributions and energy to recoil can be obtained.

Results and Discussions

The data is obtained through the simulations of the SRIM and TRIM software with TRIM running the simulation for type *Details Calculation with Full Damage Cascades*. Table 1 shows the rate of energy loss (dE/dx) for ions together with the penetration data at incidence energy 100 keV and 1000 keV respectively. The parameters that give effect to the formation of radiation damage are the ion mass, ion species, the target temperature during irradiation, total dose, ion's energy and the ion's fluence (number of ions per unit area).

Table 1. Stopping Power and Penetration Range of Helium Ion in Gallium Arsenide

Ion Energy (keV)	dE/dx Elec (keV/μm)	dE/dx Nuclear (keV/μm)	Projected Range (μm)	Longitudinal Straggling (μm)	Lateral Straggling (μm)
100	3.895E-01	6.637E-03	0.5055	0.1863	0.1793
1000	6.921E-01	1.232E-03	3.020	0.3165	0.4089

Based on Table 1, it is observed that as the energy of the helium ion increases, the projected range or depth of penetration and the distribution of the ions in Gallium Arsenide also increases. The electronic stopping power of helium ion also increases with increasing ion energy, whereas the nuclear stopping power decreases with increasing ion energy. From Table 2, it is observed that the penetration range and the dispersion of the ion for all coordinates of longitudinal, lateral and radial for all angles undergo a very small change not exceeding $0.02\mu\text{m}$. This can be inferred that even with increasing number of ions penetrating the atom, the penetration depths are almost the same.

Table 2. Depth of Ion Penetration in Gallium Arsenide at incidence energy of 100 KeV

Angle of Incidence	No. of Ions	Penetration Range (μm)			Dispersion (Straggle) (μm)		
		Longitudinal	Lateral	Radial	Longitudinal	Lateral	Radial
0°	100	0.4914	0.1697	0.2489	0.1589	0.2041	0.1184
	10000	0.5029	0.1531	0.2407	0.1448	0.1897	0.1164
60°	100	0.2916	0.4449	0.4850	0.1245	0.4715	0.1479
	10000	0.2920	0.4360	0.4801	0.1403	0.4631	0.1389

Fig.1 to Fig. 3 shows the dispersion plot of 100 helium ions in GaAs at incidence energy of 100 keV at 0° from x, y and z view respectively.

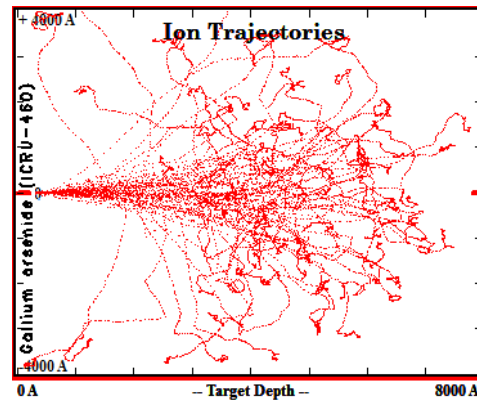


Figure 1: Dispersion of ions at axis X against Y at $E_{He}=100\text{ keV}$ at 0°

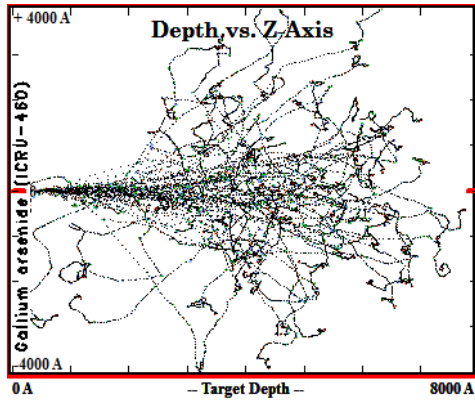
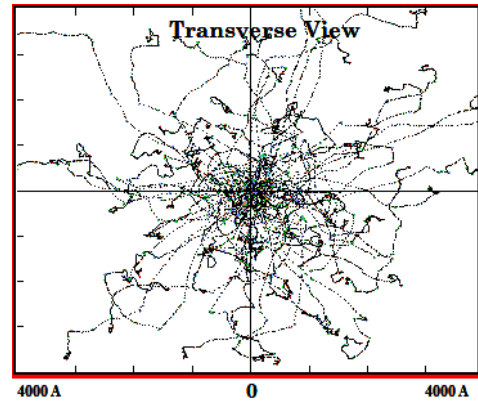
Figure 2: Depth vs Z Axis at $E_{He}=100$ keV at 0° Figure 3: Transverse view at $E_{He}=100$ keV at 0°

Fig. 4 to Fig.6 shows the dispersion plot of 100 helium ions in GaAs at incidence energy of 100 keV at 60° from x, y and z view respectively.

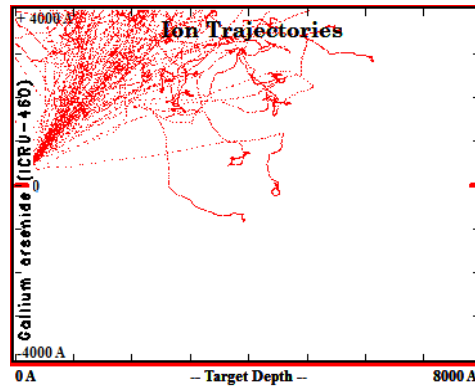
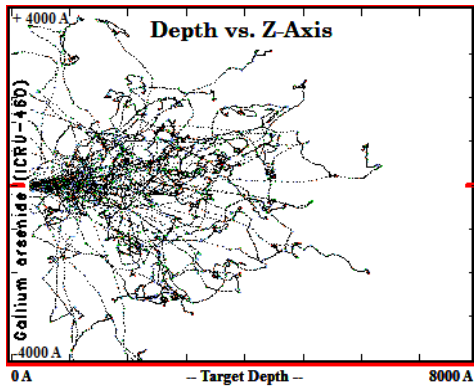
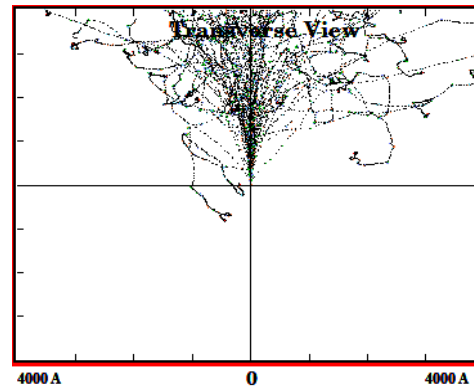
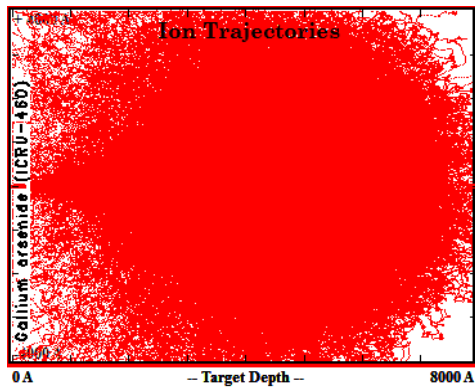
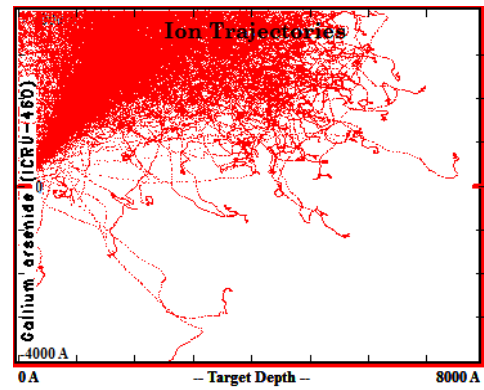
Figure 4: Dispersion of ions at axis X against Y at $E_{He}=100$ keV at 60° Figure 5: Depth vs Z Axis at $E_{He}=100$ keV at 60° Figure 6: Transverse view at $E_{He}=100$ keV at 60°

Fig. 7 and Fig. 8 show the ion trajectories of 10,000 helium ions in GaAs at incidence energy of 100 keV at 0° and 60° respectively.

Figure 7: Ion trajectories at $E_{He}=100$ keV at 0° Figure 8: Ion trajectories at $E_{He}=100$ keV at 60°

The dispersion plots show that even as the number of ions penetrating the atom increases, the dispersion and depth of penetration of the ion is about the same but with the number of Helium ions and recoil atoms to be more densely packed together.

Based on Table 3, the depth of penetration of the ion will decrease as the angle of incidence increases for all number of ions. The dispersion plots also show that when the angle of incidence of the Helium ions increases, the ions that penetrate Gallium Arsenide disperse closer to the surface of Gallium Arsenide compound atom which is at the X axis and thus there will be less penetration.

Table 3. Depth of Ion Penetration in Gallium Arsenide (Energy of ion is 1000 KeV)

Angle of Incidence	No. of Ions	Penetration Range (μm)			Dispersion (Straggle) (μm)		
		Longitudinal	Lateral	Radial	Longitudinal	Lateral	Radial
0°	100	3.05	0.2668	0.4569	0.2034	0.3337	0.2599
	10000	3.01	0.3182	0.4990	0.2705	0.4121	0.2941
60°	100	1.59	2.59	2.61	0.3367	2.60	0.2718
	10000	1.51	2.61	2.64	0.3686	2.62	0.2897

Fig. 9 and Fig. 10 show the transverse view of 100 helium ions in GaAs at incidence energy of 1 MeV at 0° and 60° respectively.

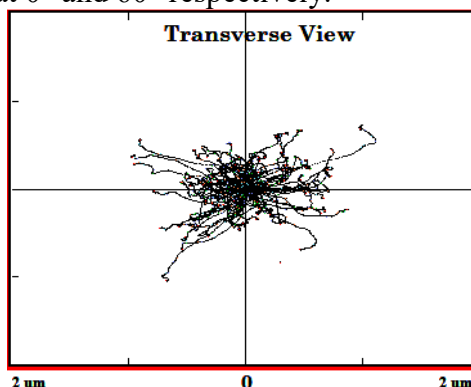
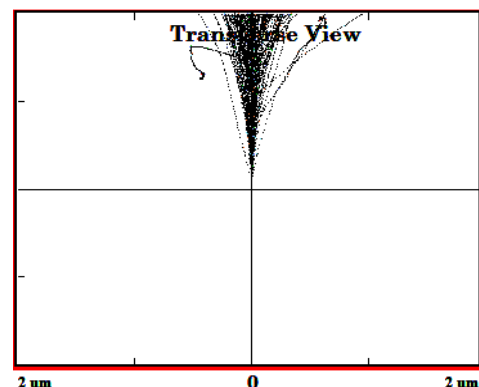
Figure 9: Transverse view at $E_{He}=1$ MeV at 0° Figure 10: Transverse view at $E_{He}=1$ MeV at 60°

Fig.11 and Fig. 12 show the Z-axis view of 10000 helium ions in GaAs at incidence energy of 1 MeV at 0° and 60° respectively.

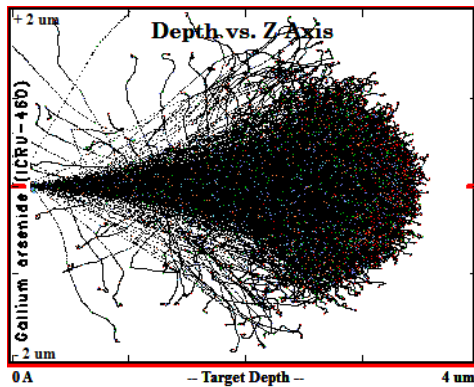


Figure 11: Depth vs Z axis at $E_{He}=1$ MeV at 0°

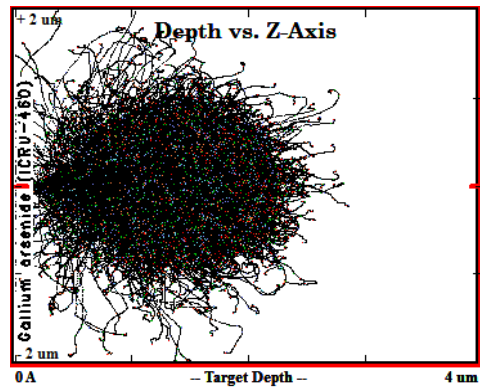


Figure 12: Depth vs Z axis at $E_{He}=1$ MeV at 60°

Conclusion

Based on the analytical discussion, it is found that an increasing angle of incidence causes the depth of penetration of helium ions to decrease and also a small fluctuating pattern for the number of damages produced per helium ion toward the GaAs. The increase of the number of helium ions shows an increase of density of lattice damage and cause the Gallium Arsenide lattice to suffer severe damages. Thus it can be concluded that the varying energy of helium ions, the incidence angle, and number of penetrating ions affects the movement and mechanism of penetration of helium ion in Gallium Arsenide compound.

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