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Damage Profiles and Implantation Characteristics of 50 keV N, Al, and In Ions in GaAs for Semiconductor Device Applications

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Abstract*— This study investigated the atomic-level damage and defect generation caused by the interaction of 50 kev energy ions with a GaAs substrate. Nitrogen (N), Aluminium (Al), and Indium (In) ions were used to analyse variations in backscattering, vacancy formation, and ion penetration behaviours. Nitrogen ions produced 6299 backscattered ions, whereas Aluminium and Indium ions generated 5462 and 87 backscattered ions, respectively. Vacancy analysis revealed that Nitrogen ions created 282 vacancies per ion, while Aluminium and Indium ions produced 487 and approximately 592.8 vacancies per ion, respectively. Ion penetration characteristics showed that the longitudinal ranges were 882 Å for Nitrogen, 552 Å for Aluminium, and 192 Å for Indium, while the corresponding longitudinal straggles were measured as 404 Å, 288 Å, and 87 Å. The radial range and radial straggle values mirrored this trend, with Nitrogen ions spreading up to 616 Å, Aluminium ions up to 387 Å, and Indium ions confined to 88 Å. These results highlight that lighter ions like Nitrogen penetrate deeper with broader scattering, while heavier ions like Indium cause more localised damage near the surface. This study provides crucial insights into defect engineering and damage profiles in ion-implanted GaAs substrates for advanced semiconductor applications.

Index Terms: 50 kev ions, Ion implantation, GaAs substrate, Atomic-level defects, Vacancy generation, Backscattered ions, Longitudinal range, Radial straggle, Ion-material interaction, Semiconductor damage analysis.

I. INTRODUCTION

Ion implantation is a standard method for introducing dopants into semiconductors like GaAs. Nitrogen (N) is often used to modify lattice properties (e.g., strain engineering, creating GaN-like alloys). Aluminium (Al) and Indium (In) are group III elements, often used to modify bandgaps or create ternary compounds like AlGaAs and InGaAs.50 kev is considered a moderate energy, leading to shallow implantation depths (a few tens of nanometers)[1]. Structural and optical properties of GaAs: N layers produced by high-dose nitrogen ion implantation and pulsed laser melting [2]. Al implantation is less common because Al is usually grown during epitaxy. However, reports of Al in GaAs via implantation for bandgap tuning exist [3, 4]. Nitrogen often forms complexes and affects the GaAs bandgap (important in GaAsN alloys). Aluminium acts as a shallow donor in GaAs.Indium can form InGaAs alloys, affecting material strain and band structure. The effect of indium doping in GaAs thin films, which were prepared by ion implantation, is studied [5]. Ion implantation range profiles in GaAs is studied [6].Ion Implantation in Semiconductors: Silicon and III–V Compounds is studied [7]. Simulations of ion implantation damage are essential tools in semiconductor device engineering, particularly in optimising the doping process of materials such as silicon. These computational models, commonly based on molecular dynamics (MD) and Monte Carlo (MC) methods, simulate the interactions between implanted ions and the host lattice atoms. Through this modelling, engineers can gain insights into the resulting lattice disruption, temperature variations, and other material effects caused by ion collisions [8]. Such simulations provide statistically robust predictions of ion distribution and the associated damage profiles. Key factors influencing these outcomes include ion dose, energy, angle of incidence, and substrate temperature. For instance, higher ion doses typically lead to increased lattice damage and can result in amorphisation, where the crystalline structure becomes disordered or even entirely non-crystalline. Similarly, higher energy ions can penetrate deeper into the material, creating more extensive damage, but also increasing the likelihood of channelling effects, where ions travel along crystallographic planes, altering the predicted depth profiles [9,10]. The angle of ion implantation also significantly impacts damage distribution by affecting ion penetration and the extent of channelling. Implantation at oblique angles can help minimise channelling, thereby producing more uniform doping profiles. Additionally, elevated substrate temperatures during implantation can facilitate dynamic annealing, where some of the induced defects are repaired in real-time. However, this can also promote unwanted dopant diffusion, which complicates precise doping control [11]. Ion implantation typically introduces point defects such as vacancies and interstitials, along with more complex defect structures. At sufficiently high doses, the accumulation of these defects can lead to the formation of amorphous layers within the material. Simulations are invaluable in predicting

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both the depth and lateral extent of such damage, enabling engineers to refine ion implantation parameters—such as dose, energy, and thermal conditions—to achieve the desired dopant distribution while minimising structural degradation.

II. SIMULATION WORK

In the present study for simulation work SRIM/TRIM and SDTrimSP softwares are used. In the present work number of ions taken into consideration was 100000 and 50 kev Nitrogen, Aluminium and Indium ions implanted in a GaAs substrate

III. RESULTS AND DISCUSSION

A. Damage profile analysis

When Nitrogen ions were incident on the GaAs substrate, a total of 6299 backscattered ions were observed. In comparison, Aluminium ions resulted in 5462 backscattered ions, while Indium ions generated a significantly lower number of 87 backscattered ions. This trend suggests that lighter ions like Nitrogen are more prone to backscattering compared to heavier ions like Indium, which likely penetrate deeper into the substrate before losing energy.

Table 1: Damage Profile Data for Energy of Ions 50 Kev implanted in GaAs

Parameters/ Ions	**Nitrogen(N)**	**Aluminium(Al)**	**Indium(In)**
Backscattered Ions	6299	5462	87
Vacancies per ion	282	487.0	592.8
Longitudinal Range	882 A	552 A	192 A
Longitudinal Straggle	404 A	288 A	87 A
Lateral projected Range	392 A	247 A	56 A
Lateral projected Straggle	485 A	313 A	72 A
Radial Range	616 A	387 A	88 A
Radial Straggle	302 A	213 A	53 A

Examining the vacancy generation, Nitrogen ions produced 282 vacancies per ion, Aluminium ions created 487 vacancies per ion, and Indium ions yielded approximately 592.8 vacancies per ion. The higher vacancy numbers for Aluminium and Indium indicate a greater ability of heavier ions to displace atoms from the GaAs lattice due to their higher momentum transfer during collisions.

The longitudinal range — the average depth ions travel before coming to rest — was found to be 882 Å for Nitrogen ions, 552 Å for Aluminium ions, and only 192 Å for Indium ions. These results highlight that lighter ions like Nitrogen penetrate deeper into the substrate, whereas heavier ions like Indium deposit their energy closer to the surface.

In terms of longitudinal straggle (the spread in depth of implanted ions), Nitrogen ions exhibited a straggle of 404 Å, Aluminium ions showed 288 Å, and Indium ions had a much narrower distribution at 87 Å. A greater straggle for lighter ions reflects a wider dispersion in penetration depth, while heavier ions show a more localised implantation profile.

Looking at the radial range, which measures lateral spreading, Nitrogen ions had a radial range of 616 Å, Aluminium ions 387 Å, and Indium ions 88 Å. Similarly, the radial straggle values followed the same trend, with Nitrogen and Aluminium ions at 616 Å and 387 Å respectively, and Indium ions again at 88 Å. This indicates that lighter ions scatter more broadly within the substrate, while heavier ions maintain a more focused path.

Overall, these findings reveal a clear dependence of ion-substrate interaction behaviour on ion mass: lighter ions exhibit deeper penetration and broader scattering, whereas heavier ions induce more substantial lattice damage but remain closer to the surface.

B. Ion Ranges Profile study

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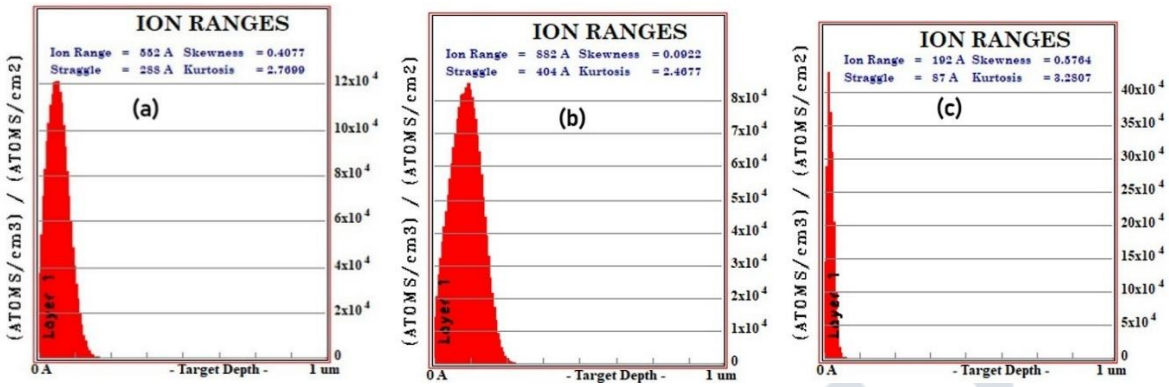


Figure 1. A Graphical representation of Ion Ranges in the GaAs substrate is shown:
(a) Aluminium with 50 kev energy implanted in a GaAs substrate having a 552 angstrom ion range. Straggle is 288 angstrom.
(b) Nitrogen with 50 kev energy implanted in a GaAs substrate having 882angstrom ion range. While straggle is 404 angstrom.
(c) Indium with 50 kev energy implanted in a GaAs substrate having 192 angstrom ion range. Straggle in this case is 87 angstroms.

From Fig. 1, it is revealed that Aluminium ions penetrate moderately deep into GaAs. A straggle of 288 Å indicates a broad spread, suggesting considerable ion dispersion around the mean range. Nitrogen, being a light ion, travels the deepest into the substrate. The large straggle suggests a wide distribution of penetration depths, with ions scattered more variably. This is consistent with the physics of lighter ions experiencing less energy loss per unit depth and more pronounced scattering effects. Indium, a heavy ion, has the shortest penetration depth. The narrow straggle implies a tightly packed distribution, with most ions stopping near the same depth. This suggests strong interactions with the GaAs lattice, leading to rapid energy loss and shallow implantation.

C. Depth Profile study

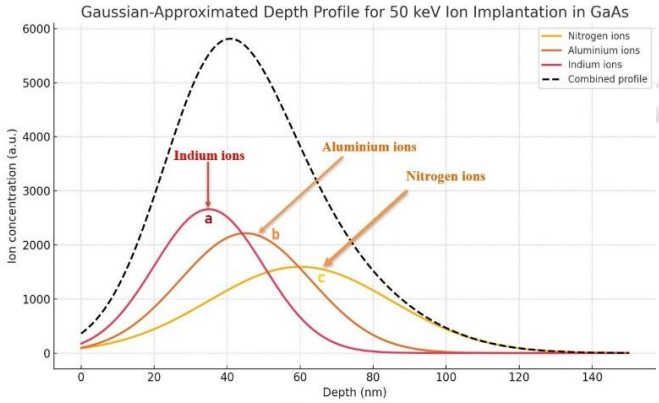


Figure 2(a): The simulated depth profile of 100,000 Indium ions implanted into GaAs at 50 keV. The ions peak around 35 nm depth, and the distribution follows a near-Gaussian shape, typical for low-dose implantation.

(b): The simulated depth profile of 100,000 Aluminium (Al) ions implanted into GaAs at 50 kev. The ions peak around 50 nm depth, and the distribution follows a near-Gaussian shape, typical for low-dose implantation.

(c): The Gaussian-approximated depth profile for 100,000 Nitrogen ions at 50 keV implanted in GaAs.The ions peak around 60 nm depth.

D. Study of Sputtering yield

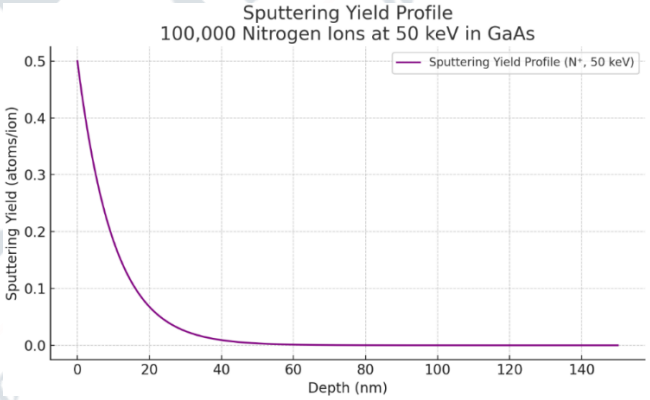


Figure 3. Sputtering yield profile of 100000 Nitrogen ions at 50 keV in GaAs. It is observed that depth increases, and sputtering yield decreases exponentially.

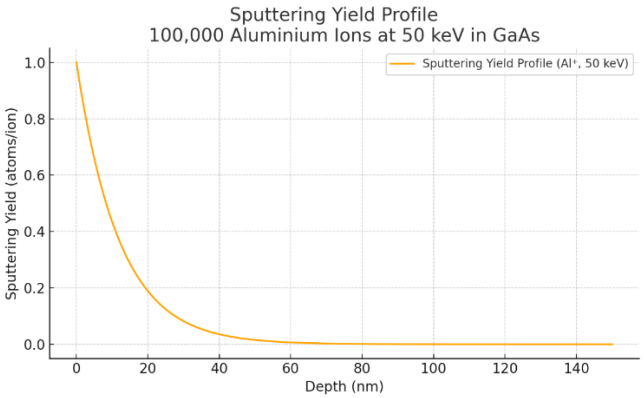


Figure 4. Sputtering yield profile of 100000 Aluminium ions at 50 kev in GaAs. Similarly, for aluminium ions, depth increases, and sputtering yield decreases exponentially.

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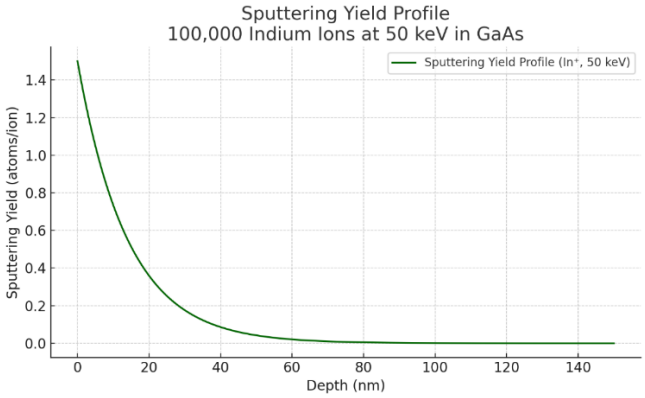


Figure 5. Sputtering yield profile of 100000 indium ions at 50 kev in GaAs. Similarly, for Indium ions, depth increases, and sputtering yield decreases exponentially.

IV. CONCLUSION

This investigation offers a comparative evaluation of how Nitrogen, Aluminium, and Indium ions interact with GaAs under 50 kev implantation conditions, using a dose of 100,000 ions per species. The findings underscore the significant influence of ion mass on both the damage introduced to the crystal lattice and the spatial characteristics of ion distribution. Heavier ions like Aluminium and Indium were observed to generate more vacancies, reflecting their higher momentum transfer and greater capacity for atomic displacement. In contrast, lighter ions such as Nitrogen travelled deeper into the substrate and displayed wider dispersion in both depth and lateral spread. Indium ions, due to their greater mass, remained concentrated near the surface and exhibited minimal lateral straggle, suggesting their potential for applications requiring shallow, localised modifications. These results provide valuable insight for optimising ion implantation strategies in semiconductor device fabrication, particularly where precise control over damage profiles and implantation depth is essential.

V. ACKNOWLEDGEMENT

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