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Study of damage profiles and energy calculation of arsenic ions during ion implantation on Germanium

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ABSTRACT

Computational calculation of energy loss and damage profiles when implanted by arsenic ions on amorphous germanium during ion implantation had been carried out. The required energies for doping of arsenic ion on germanium, in order to obtain maximum damage at 600 Å, were calculated using SRIM. These ions when implanted on germanium causes the production of germanium recoils, vacancy-interstitial pairs, and phonons during the collision process. For 140 keV arsenic ion, the energy consumption for ionization, phonon production and vacancies creation are 39.634 keV (28.31% of incident energy), 90.888 keV (64.92% of incident energy) and 9.478 keV (6.77% of incident energy), respectively. The amount of target displacement, replacement collisions and vacancies were also evaluated. Doping of arsenic ions on germanium also revealed that the energy loss due to nuclear stopping was greater than electronic stopping. Significantly, surface hardness and electrical conductivity on germanium cannot be improved with calculated energies.

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1. Introduction

Ion implantation

Ion implantation is the process in which an accelerated ion allowed to enter the surface of the target material. Ion implantation method is used in semiconductor device fabrication and in metal finishing, as well as various applications in materials science research [1]. Ion implantation in semiconductors is currently receiving attention in several rather different contexts. Semiconductor physicists and device engineers are interested in the implantation process because it provides a new doping technique with several potential advantages over more conventional doping methods. Material scientists are interested in the electrical properties of ion-implanted semiconductors because they provide an important tool for studying solubility problems, diffusion processes, and radiation damage effects. And nuclear physicists are interested in the ion distribution profile in an implanted semiconductor because, among other things, it yields important information on the nature of the physical processes that occur when an energetic particle interacts with a crystalline or amorphous target [2]. This technology also has its

very strong application in medical physics for treatment of cancer using radiations e.g. proton therapy [3].

Most importantly, ion implantation requires an understanding of the fundamental physics and chemistry that dictate the interaction of the ion beam and the target. The ions alter the elemental composition of the target (if the ions differ in composition from the target), stopping in the target and staying there. They also cause many chemical and physical changes in the target by transferring their energy and momentum to the electrons and atomic nuclei of the target material [4]. This causes a structural change, in that the amorphous structure of the target can be damaged or even destroyed by the energetic collision cascades.

Nowadays this has been easier to a great extent by various simulations and programming. SRIM is one of the simulation programs based on Monte Carlo mathematical framework of quantum collision that predicts the various damages during ion implantation experiments [5]. Since ion implantation is a low temperature process, thermal effects are not considered in SRIM for calculation of damage profiles on germanium, so the damage which is calculated is that which would happen for an implantation at 0 K. Also, this paper doesn't take account of the dynamic composition changes in the material and there is no description of defect clustering and irradiation-induced amorphization that severely limits its usefulness in some cases.

Germanium as a substrate for ion implantation

The development of the germanium transistor in 1948 opened the door to countless applications of solid state electronics. From 1950 through the early 1970s, this area provided an increasing market for germanium [6]. Development in quantum physics in turn allowed the development of the integrated circuits in 1958 [7] and the transistor in 1947 [8]. Meanwhile, the demand for germanium for fiber optic communication networks, infrared night vision systems, and polymerization catalysts increased dramatically.

Solar panels are a major use of germanium. Germanium is the substrate of the wafers for high-efficiency multi junction photovoltaic cells for space applications. High-brightness LEDs, used for automobile headlights and to backlight LCD screens, are an important application. Because germanium and gallium arsenide have very similar lattice constants, germanium substrates can be used to make gallium arsenide solar cells. Germanium-on-insulator substrates are seen as a potential replacement for silicon on miniaturized chips [9]. The Mars Exploration Rovers and several satellites use triple junction gallium arsenide on germanium cells [10]. Other uses in electronics include phosphors in fluorescent lamps and solid-state light-emitting diodes (LEDs) [11]. Germanium transistors are still used in some effects pedals by musicians who wish to reproduce the distinctive tonal character of the "fuzz"-tone from the early rock and roll era, most notably the Dallas Arbiter Fuzz Face [12]. Presently, the major end uses are fibre-optic systems, infrared optics, solar cell applications, and light-emitting diodes (LEDs). Germanium compounds are also used for polymerization catalysts and have most recently found use in the production of nanowires.

Properties of germanium can be altered in useful ways by the deliberate, controlled introduction of impurities ("doping") into the crystal or amorphous structure and we take the amorphous structure as a target. Where two differently-doped regions exist in the same layer, a p-n junction is created. The behavior of charge carriers which include electrons, ions and holes at these junctions is the basis of diodes, transistors and all modern electronics [13].

Stopping power

The stopping power is an essential parameter when ions penetrate matter. It defines how much energy per unit path length an ion loses when penetrating a crystal, thus the stopping power is usually measured in units of $eVcm^{-1}$ but here we will measure the stopping power in eV/Å. The stopping power depends primarily on the type of material which is penetrated and on the ion energy.

When energetic ions are allowed to penetrate through target surface, a series of screened coulomb collision occur where the ion's energy gets divided into two stopping parameters, one is nuclear stopping and another is electronic stopping.

Mathematically, the total stopping power can be given as:

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

where, S = Total stopping power and defined as the energy loss (E) per unit path length (x) of the ion is the sum of these two factors; nuclear stopping and electronic stopping.

Nuclear stopping is the energy loss by ion to the target nuclei per unit path length of the ion. It is an elastic collision between two atoms and can be described by classical kinematics. Electronic stopping is the energy loss by ion to the electrons of target atoms per unit path. It is an inelastic collision and the theoretical model is quite complex. The stopping is similar to a viscous drag force and is proportional to the ion velocity. The energy loss by incident ions is dissipated through the electron cloud into thermal vibrations of the target. The energy loss by Electronic energy loses are more important than nuclear energy loses for improving hardness at the near-surface region. The electrical conductivity and hardness increases with the increase in electronic energy loss while, conductivity and hardness increases with the decrease in nuclear energy loss. This remarkable improvement in hardness and electrical conductivity is related to the degree of radiation-induced changes in microstructure and composition. In particular, determination of the electronic stopping power becomes crucial for studies of ion ranges and radiation damage in semiconductors.

Range distribution and collision events

The range distribution depends primarily on the energy, mass, and atomic number of the incoming ions, the mass and atomic number of target atoms, the density of the target. The total distance that the ion travels in coming to rest is called its range and the projection of this distance onto the direction of incidence is called the projected range.

Total target displacements are the number of atoms knocked off their target lattice site. A vacancy is the hole left behind when a recoil atom moves from its original site. If a moving atom strikes a stationary target atom and transfers more than its displacement energy to it, and the initial atom, after the collision, does not have enough energy to move onwards, and it is the same element as the atom it struck, then it just replaces that atom in the target and there is no vacancy created. These are termed as replacement collisions.

Displacements = Vacancies + Replacement collisions …….. (2)

When a recoil atom stops, and is not a replacement atom, then it becomes an interstitial. These may be summed as:

Vacancies = Interstitials + Atoms which leave the target volume ……. (3)

If a cascade atom leaves the target volume, it is no longer followed.

2. Methods

The doping of impurities on semiconducting elements can be processed by two ways: Diffusion and Implantation [14]. Diffusion is limiting process due to saturation limit and so, we can't make high concentrated carriers. To overcome the diffusion issues of dopants and activation of dopants in material- ion implantation or ion irradiation is the best. In general, using particle accelerators to shoot energetic ion on a material is the basic process of implantation and irradiation.

Among some trending techniques we employed SRIM to study the damage profiles of target atom when doped with different ions. Because of less error in SRIM data and availability of different updated version of this program motivates me to use SRIM for the study of damages in germanium.

Simulation methodology

We use the simulation software SRIM and MATLAB for the ion implantation germanium. The core of SRIM is a program transport of ions in matter (TRIM). When an ion penetrates the target, it undergoes a series of screened coulomb collisions displacing target atoms along the way. Basically, SRIM calculates the interactions of energetic ions with amorphous targets and presents those interactions statistically and graphically which make the implantation process easier to understand.

It can also create three-dimensional plots of the ion distribution when penetrating matter, including the

trace of defects created by the ion beam and its so-called straggle and all resulting cascades which can occur when atoms are kicked out of their lattice position, becoming an interstitial atom which can subsequently hit other lattice atoms [6].

The text data of damage profiles in exponential form as calculated by TRIM are eventually converted to numerical values using Microsoft excel and thus obtained numeric values were used in MATLAB to obtain schematic graphs of related values.

3. Results and Discussion

Energy calculations

The energy needed to implant gallium and arsenic ions independently on germanium in order to obtain peak dopants concentration at range of 600 Å were tabulated using SRIM.

Arsenic in Germanium

Target density = 5.350 g/cm^3 = 4.4371 × 10^{22} atoms/cm^3

Table 2: Energy calculation for arsenic ion.

Ion Energy (keV)	dE/dx Electrical	dE/dx Nuclear	Projected Range (Å)
80.00	17.98	159.0	366
90.00	19.07	159.4	405
100.00	20.10	159.4	444
110.00	21.08	159.2	483
120.00	22.02	158.8	522
130.00	22.92	158.2	561
140.00	**23.79**	**157.5**	**600**
150.00	24.64	156.7	640
160.00	26.58	155.9	680
170.00	28.28	155.0	719
180.00	29.80	154.0	759
200.00	32.45	152.0	838
225.00	35.28	149.5	938

The table 2 demonstrates that the exact energy required for n-type arsenic dopants to obtain maximum defects at 600 Å is 140 keV. Therefore, we can now implant 10,000 arsenic ions accelerated by applying 140 keV energy in germanium monolayer target in order to obtain maximum defects concentration at 600 Å.

Stopping power

Fig.1 demonstrates the nature of stopping power for As ions bombarded on germanium. On increasing ions energy nuclear stopping goes on increasing upto 100 keV and starts decreasing gradually, while, electronic stopping goes on gradual increase and starts dominating nuclear energy loss above 1000 keV i.e.1 MeV.

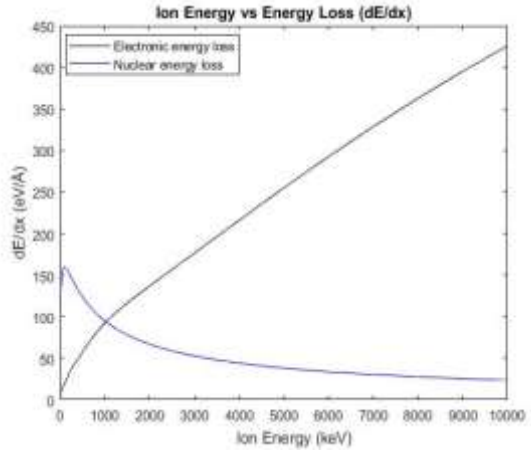

Fig. 1: Comparison of electronic energy loss and nuclear energy loss.

The point of intersection of the two curves represents the corresponding ion energy where the electronic and nuclear energy losses are equal. In addition, we can conclude that there is no improvement in surface hardening and electrical conductivity of germanium upto 1 MeV but implanting both ions above 1 MeV increases the surface hardening and electrical conductivity because of dominance of electronic stopping power and decreasing nuclear stopping power. For 130 keV gallium ions, 24.27 eV/Å and 142.60 eV/Å are the value of electronic stopping and nuclear stopping respectively. These values indicate that averagely each gallium ion lose 24.27 eV/Å to target electrons for every unit path of ion, whereas, to the target atoms, each gallium ion lose 142.60 eV/Å for every unit path of ion. Since for gallium ion accelerated at 130 keV have greater nuclear stopping so there is no improvement in surface hardness and electrical conductivity. Similarly, the value of electronic stopping is 23.79 eV/Å and nuclear stopping is 157.5 eV/Å, for 140 keV

arsenic ions. Since for arsenic ion accelerated at 140 keV have nuclear stopping, as a dominant process so desired surface hardening and electrical conductivity could not be achieved at 140 keV and similar will be for gallium ions. The reason behind dominance of nuclear stopping is mass of ions that are comparable with germanium. Comparatively, ions energy should be increased to energy above 1 MeV for both ions in order to obtain dominance of electronic stopping power over nuclear stopping power that eventually improve the surface hardening and electrical conductivity.

Energy Loss during ionization

The Fig.2 reveals the energy imparted to the target

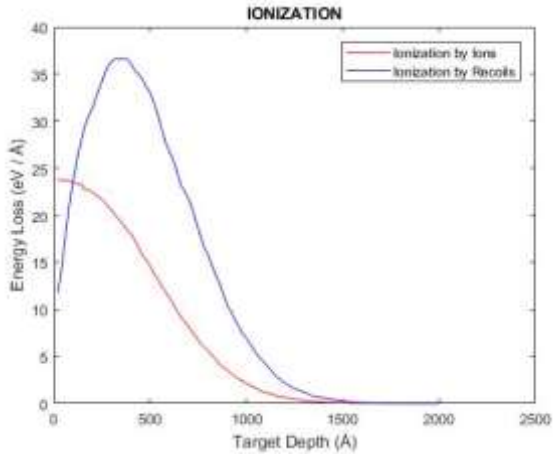

Fig.2: Energy loss distribution during ionization.

electrons during ionization process. The plot shows ionization from the incident ions and from recoiling target atoms. For both collisions, the energy loss to the target electrons by recoil atoms is greater than energy loss by ions. Maximum ionization by ions begins from the surface of the target material and then gradually falls down. Energy loss by arsenic ions and recoil atoms during ionization process is 14.126 KeV 25.508 keV respectively. And the total energy loss during ionization process during arsenic-germanium interaction is 39.634 keV.

Energy loss to phonons

When a germanium atom is knocked out of its lattice site, its binding energy,

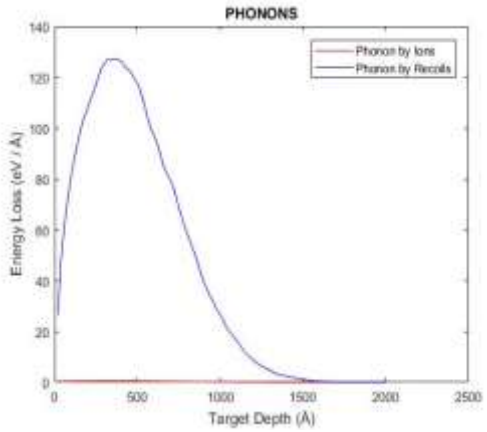

Fig. 3: Curve showing distribution of energy loss to phonons.

E_{latt} = 2 eV, is deposited into phonons produced by the recoils. Vacancies/ion for arsenic is 4371.9, therefore for each arsenic ion, displacements by the ion or recoil cascades cause 4371.9 × 2 eV= 9463.8 eV of phonons. In Fig.3, we can barely see the energy loss to phonons from the ions (red line at the bottom of the plot), and the phonons are produced almost exclusively by the recoiling target atoms. The energy loss for phonon production is high around the range of 400 Å and then the gradual fall in energy loss for phonon production occurred as we increase the target depth. For arsenic, the ions generate phonon with 0.29% of their incident energy and the recoiling atoms contribute an additional 64.63 %. It means that 0.406 keV energy is lost by ions and 90.482 keV energy is lost by recoil Ge atoms. Total energy loss to phonons arsenic-germanium interaction is 90.888 keV. Actually, phonons do not have contribution in improving electrical conductivity but do have contribution in increasing temperature of target material during implantation process.

Energy to recoil

Distribution of energy to recoil gives us the information about the amount of energy loss by ions to the recoiling atoms. Overlapping of black and yellow curves demonstrates that energy losses by ions are very absorbed by target atoms, for both ions. In Fig.4, we find that 160 eV/ion was absorbed by germanium at the surface of the target

atom followed by increase in energy loss to near 180 eV/ion at 500Å.

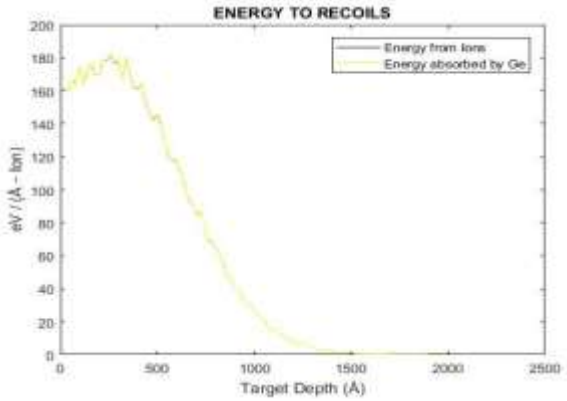

Fig. 4: Energy to recoil**.**

Ion range

Fig.5 is the curve of range distributions of ions building up in germanium target. The higher moments of the distribution (straggle, skewness, and kurtosis) are also given in the plot. Both plots have ordinate unit: "(atoms/cm^3) / (atoms/cm^2). Although these units appear strange, when we multiply by an implantation dose (ions/cm^2), we will end with the impurity concentration (atoms/cm^3) vs. depth. Plot is the distribution of arsenic

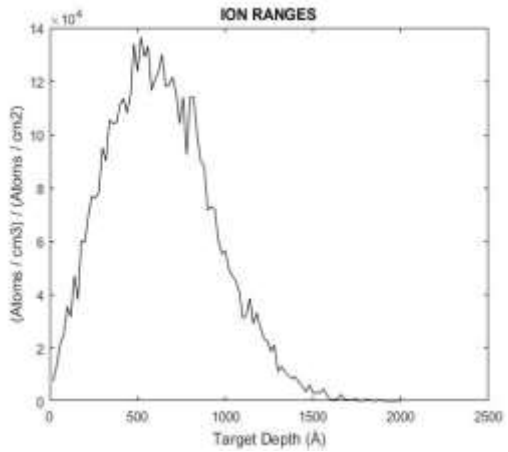

Fig. 5: Ion range distribution curve.

ions (140 keV) over germanium monolayer surface. Target depth is taken upto 1500 Å in order to catch maximum number of ion in the plot.

According to table 3, the mean ranges of implanted ions were found to be 622 Å for arsenic ion. This value show little discrepancy with the value given by SRIM. However, 600 Å was the mean ion range

Table 3: Mean range and moments.

	Arsenic
Ion Range	622 Å
Straggle	294 Å
Skewness	0.63705
Kurtosis	-25.5672

value tabulated by SRIM and as per TRIM; the value was 622 Å, for arsenic ion. This difference in mean ion range value was found as error. Therefore, the percentage error for arsenic-germanium interaction was found to be 3.67%. These discrepancies were responsible for skewness. Also, this value indicates that the peak concentrations of defects are formed at range of 622 Å for 140 keV accelerated arsenic ion.

Recoil distribution

In Fig.6, it can be seen that the concentration of recoil atoms at the surface of the target is

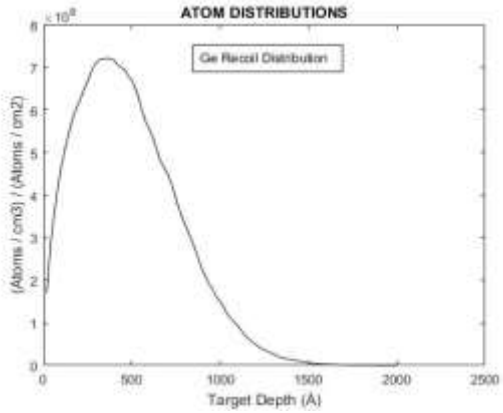

Fig. 6: Germanium recoil distribution curve.

1.8×10^8 atoms/cm^2 for arsenic-germanium collision, followed by increase in maximum concentration of recoil atoms to 7.2×10^8 atoms/cm^2 at 400 Å.

Table 4: Longitudinal, radial and lateral Projection range for As ions

	Range (Å)
Longitudinal	622
Lateral Projection	201
Radial	314

From the table 4, the average value of lateral projected for As ion is 201 Å. The radial range is 314 Å which is the mean radial displacements range from the x-axis assuming cylindrical symmetry.

Collision Events

Target displacement

The results for the collision events of the As ions with Ge target give the total target displacements as shown in Fig.7. The area under the curve gives the values for total displacements of 5116/ion arsenic.

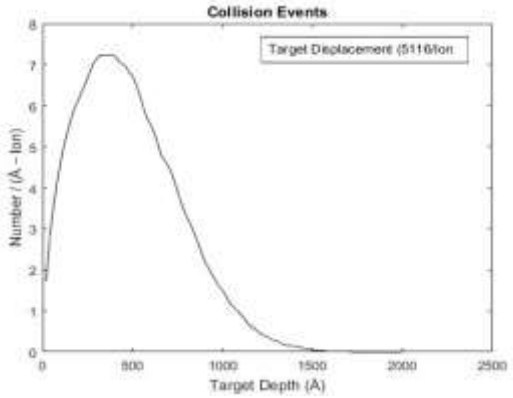

Fig. 7: Curve showing target displacement.

Target vacancies

Fig.8 shows the vacancy-target depth distribution curve which is the result of removal of Ge atoms from their equilibrium positions because of the collision process. The general feature of the curves is also similar to those of the recoil distributions in peak positions except that their magnitudes are different. Each displacement collision will lead to a displacement of a Ge atom, that resides at the end as an interstitial, and creation of a vacancy (Frenkel pair).

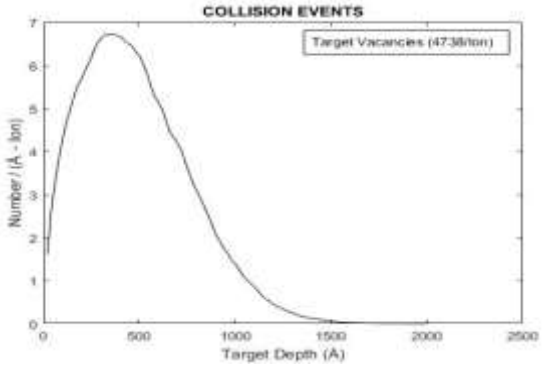

Fig. 8: Curve showing vacancies per ion.

Therefore, it is expected that the number of vacancies and interstitials produced per ion are the same. The total number of vacancies amounted to 4738/ion for As ions.

Replacement collision

The results indicate that replacement collisions of 378/ion are calculated from the collision of As ions with Ge atoms. The replacement collisions amount to 7.98% for As ions. A summary of the collision events is shown in Table 6.

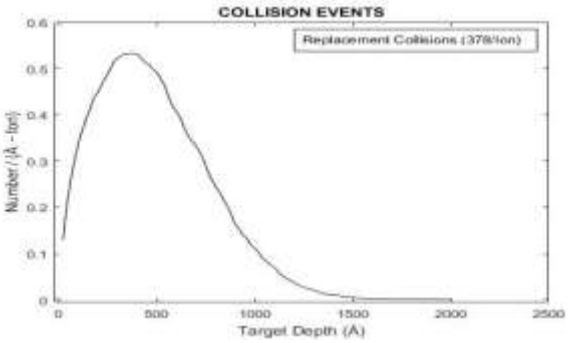

Fig. 9: Replacement collision curve.

Table 6: Defects produced during ion implantation of As in Ge.

	Arsenic
Target displacements/ion	5116
Vacancies/ion	4738
Interstitials/ion	4738
Replacement collisions/ion	378

For arsenic-germanium collision, sum of vacancies/ion and replacement/ion is equal to target displacement/ion which shows a fair agreement with equation (2).

i.e. 5116/ion = 4738/ion + 378/ion

The results presented in the figures belonging to energy loss by ionization, recoil collisions, displacement collisions, and vacancies are similar by nature of graph but are characterized by difference in their numerical values.

4. Conclusion

Doping of arsenic ions on germanium reveals that most of the energy loss is due to ionization and phonons production. For 140 keV arsenic ion, the energy loss for ionization, phonon production and vacancies creation are 39.634 keV (28.31% of incident energy), 90.89 keV (64.92% of incident energy) and 9.478 keV (6.77% of incident energy), respectively. Almost three fold amount of energy was lost during phonon production when As ions are implanted on germanium.

The collision events revealed the formation of interstitial vacancy pairs 4738, target displacements of 5116/ion and replacement collisions of 378/ion. Another important finding of this work is that we cannot improve electrical conductivity and hardness of germanium by implanting 140 keV arsenic ions. To improve these properties by implanting arsenic ions we need to accelerate these ions above 1 MeV of energy.

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