Journal of Ovonic Research Vol. 15, No. 3, May – June 2019, p. 167 - 172

DEFECT PROFILE SIMULATION OF OXYGEN IMPLANTION INTO Si AND GaAs

N. DAHBI[a*], R. B. TALEB [a], O. ZAOUI [a]
[a]*Laboratory of Semiconductor Devices Physic, University of Tahri Mohamed, PB 417, Bechar (08000), Algeria*

This study concerns the ion implantation of oxygen in two semiconductors Si and GaAs realized by a simulation using SRIM tool. The goal of this study is to compare the effect of implantation energy on the distribution of implant ions in the two targets and to examine the different processes resulting from the interaction between the ions of oxygen and the target atoms (Si, GaAs). SRIM simulation results indicate that the implanted ions have a profile as a function of Gaussian-type; oxygen produced more vacancies and implanted deeper in Si compared to GaAs. Also the most of the energy loss is due to ionization and phonon production, where vacancy production amounts to few per cent of the total energy.

(Received January 16, 2019; Accepted May 11, 2019)

Keywords: Defect profile; Ion implantation; SRIM; Phonon production; Vacancies.

1. Introduction

Ion implantation is a very common method for doping semiconductor materials since the doping profile is easily controlled compared to dopant diffusion methods. The very same technique can be used to bombard material with ions to electrically isolate them [1]. Ion implantation represents a particularly useful means by which to modify the surface properties of a variety of materials. This prosaic statement, however, does not convey the depth of basic understanding which has been developed to fully utilize the advantages of ion implantation. The interaction of a host lattice with the energetic beams produces metastable states and structures which cannot be achieved by other means. However, ion implantation also requires an understanding of the fundamental physics and chemistry that dictate the interaction of the ion beam and the target. In addition to the fundamental nature of the process, ion implantation is important to a wide variety of technologies [2] and it is a process that introduces ionized-projectile atoms into targets with enough energy to penetrate beyond surface regions [3].

Gallium arsenide is a widely used semiconductors materials that offer decisive advantages to silicon and germanium for some opto-electronic applications and during the preparation of GaAs or Si thin films, oxygen is presented and it has an influence on the electrical and optical properties of these semiconductors [4].

Because ion implantation is usually the best means to introduce dopants into materials in a controlled manner [5], the interest in understanding the effects of oxygen ion presence in GaAs and Si is important for the further development of controlled manufacturing of these materials. However, implantation cannot be done without the introduction of radiation damage into the sample. Ions, which are propelled into the substrate crystal, collide with substrate atoms and displace them from their lattice sites in large numbers [6].

If lighter ions relative to the masses of the host atoms of the material are implanted, collision cascades are very dilute and consist mostly of point defects such as vacancies and interstitials [7]. In the case ofeavy ions, where the nuclear energy loss rate is large, it is generally believed that each ion generates a dense collision cascade which, upon very fast quenching an often result in an amorphous zone [8]. Irradiation by an intermediate mass ion represents a combination of these two limiting cases [7].

---

*Corresponding author: algiriarose@yahoo.com

Once defects are formed by incident ion, those defects will reorder to form more stable configurations. For example, the vacancy in silicon is an unstable defect and is quite mobile at room temperature. After vacancies are introduced, they move through the lattice and form more stable defects. The effectiveness of defects in altering the properties of bulk semiconductor material and devices depends on the nature of the specific defects and on the time after defect creation at a given temperature. In general, any disturbance of lattice periodicity may give rise to energy levels in the band gap. Radiation-induced defects have such levels associated with them, and it is these defect states, or centers, that have a major impact on the electrical and optical behavior of semiconductor materials and devices. The basic phenomena that cause materials and devices to degrade in a radiation environment that produces displacement damage are: 1) incident particles displace atoms; 2) the resulting defects give rise to new energy levels; and 3) those levels alter material and device electrical and optical properties [9].

We propose in this work a numerical simulation study of the oxygen implantation effect on GaAs compared with Si, according the Stopping and Range of Ions in Matter (SRIM) software, in order to investigate the defect profile, ionization phenomena and phonon production.

2. SRIM simulation

The interaction between incident ions and target atoms is composed of two mechanisms: one is the interaction between ions and the nucleus of the target atoms and another is the interaction with the electrons of the target atoms, which are treated as independent mechanisms. These mechanisms can be directly implemented into Monte Carlo simulation such as SRIM [9].

Stopping and Range of Ions in Matter or SRIM is a collection of software packages developed by Ziegler and Biersack that calculate the stopping and range of ions into matter [10]. SRIM is a reference and extremely popular program in the radiation effects community; it is based on a Monte Carlo simulation method, namely the binary collision approximation with a random selection of the impact parameter of the next colliding ion. Among all functionalities of the developed packages, SRIM includes quick calculations that produce tables of stopping powers, range and straggling distributions for any ion at any energy (in the range 10 eV–2 GeV) and in any elemental target. More elaborate calculations include targets with complex multi-layer configuration [11].

A special independent executable program called TRIM is included with SRIM; this is a program which can be used as a subroutine for other applications which require ion stopping powers or ranges. TRIM (The TRansport of Ions in Matter) a widely used computer code can always predict the atomic profile and damage distribution, which can be compared with actual measurements of the atomic profile using Secondary Ion Mass Spectroscopy (SIMS). The program may accept complex targets made up of compound materials, with up to three layers made up of different materials. It will calculate both the final distribution of the ions and also all kinetic phenomena associated with the energy loss of the ion, such as target damage, ionization, and phonon production. All target atom cascades in the target are followed in detail, and the redistribution of these target atoms is determined [10][12].

3. Results and discussion

In order to investigate the effect of the presence of oxygen in 2 µm GaAs and Si thick films, 5000 ions incident at zero degree of Gallium Arsenide and Silicon target surface are used with a variant implantation energy from 100 Kev to 1Mev.

3.1. Implantation energy dependence

When ions are implanted into the material, collision cascade occur during the implantation process this effect may cause abundant defects. Generally speaking, the collision has three independent processes, including nuclear collision, electron collision, and charge exchange.

Among of these, nuclear collision pertains to elastic collision, and the result is that abundant defects will be created [13]. A comparison of the vacancies number produced by oxygen ions bombardment of GaAs and Si as a function of implantation energy is been shown in Fig. 1. It is clear that, by increasing the implantation energy the number of vacancies increases and the oxygen implantation produces more vacancies in Si target compared with GaAs target, which prove the good irradiation resistivity of GaAs.

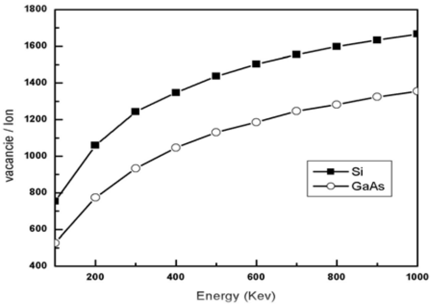


Fig. 1.Vacancies produced from oxygen implantation as a function of implantation energy, estimated by SRIM calculations.

When discussing the range of the implanted ions a common term is the projected range, R_p, which is defined as the projection of the range in the direction of the incoming energetic ions. Since the stopping process is stochastic and not all ions experience the exact same stopping forces, nor deflect at the same angle in collisions, all ions will not end up in the same place. This leads to a certain spread in R_p, this spread is defined as straggle of the projected range [14].

Fig. 2 below presents a plot of projected range as a function of ions energy for oxygen ions implanted into GaAs compared with Si. It can be seen from this plot; that the oxygen ions penetrate in Si deeper than in GaAs, also when the implantation energy is increasing the ion range also increase.

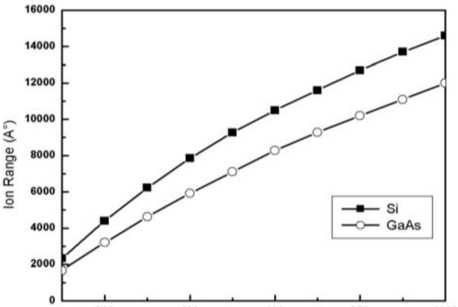
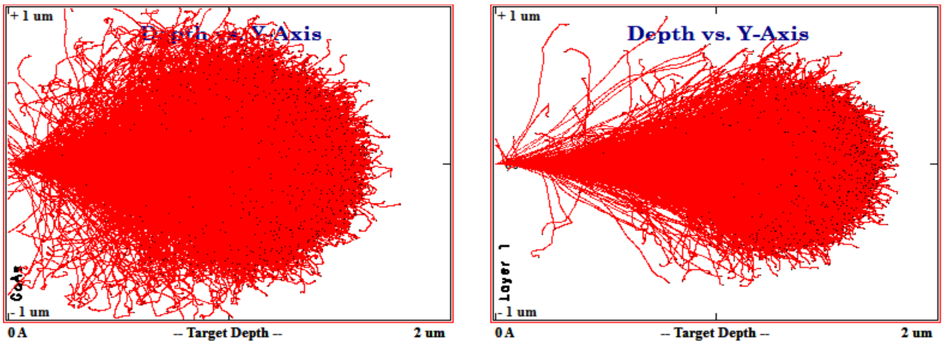


Fig.2.Ion range as a function of implantation energy for oxygen implantation, estimated by SRIM calculations.

3.2. Cascade collision

We used the SRIM software to determinate the penetration depth and spatial distribution of O^{-} ions in GaAs and Si materials. Whenever an ion undergoes a nuclear collision with the target atoms (GaAs, Si), part of its initial energy is transferred to the nucleus of the atoms-target, if the value of this energy is greater than binding of the target atom, this one leaves its site and moves in the material, constituting in its turn a projectile. Electron collision refers to the collision between incident ions and electrons of the target material, and this collision process pertains to an inelastic collision process. During the electron collision process, electrons of target atoms will probably be excited. During this process, incident ions transfer energy to target atoms or electrons of target atoms, and the incident ions will be stopped within the target after multiple impacts[10][13]. Fig. 3 shows the process of cascade collision of 1 Mev implantation into GaAs and Si, it is clear that the ions collisions occupy large region of our targets.

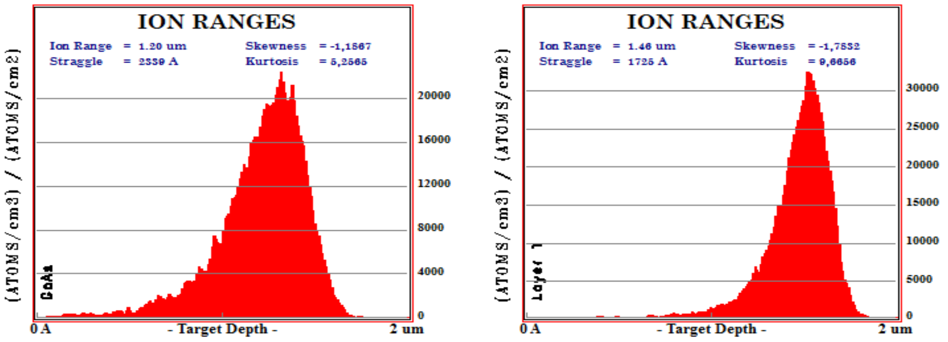


(a) *(b)*

Fig. 3. SRIM ions trajectories for 1MeV O^{--} ions in: (a) GaAs, (b) Si.

3.3. Ion distribution

The ions distribution in GaAs and Si layers is illustrated in Fig.4, which indicates that the implantation profile is constructed using the depth, the distribution in the transverse plane is Gaussian-type beam particles. When we bombard GaAs target with 1 Mev oxygen ions, we find that ion ranges reach to 1.20 um and the straggle equal to 2559 A, while in the Si target, the oxygen ions penetrate deeper and the ions ranges reach to 1.46 um, where the straggle get 1725 A.



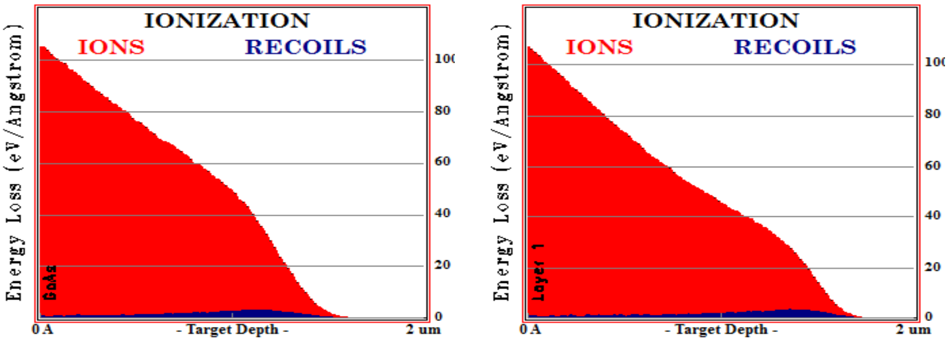
(a) *(b)*

Fig.4. Depth profile simulated by SRIM of 1 MeV O^{--}ions implanted into: (a) GaAs, (b) Si.

3.4. Ionization process

The main effect of the introduction of 1 MeV accelerated oxygen ions as well as the recoiled ions in the surface is the ionization process. Ionization is energy loss to the target electrons; the electrons of the target absorb energy from the fast moving ions and recoil atoms, and then release it as heat if the target is a metal or as phonons if the target is an insulator. The plot in Fig.5 shows ionization from the incident ions (O^{--}) and also from recoiling target atoms.

The curves are typical of the ionization of charged particles; maximum ionization begins from the surface of the target material with sharp peaks. Area under the curve calculations for the ions and the recoils show that the oxygen ions loss is about (88.73%) its energy in the ionization process in GaAs target; while in Si target ions loss (90.87%) from the energy. We can conclude that the ionization coming almost from ions energy loss, where the contribution of the recoil is neglected.

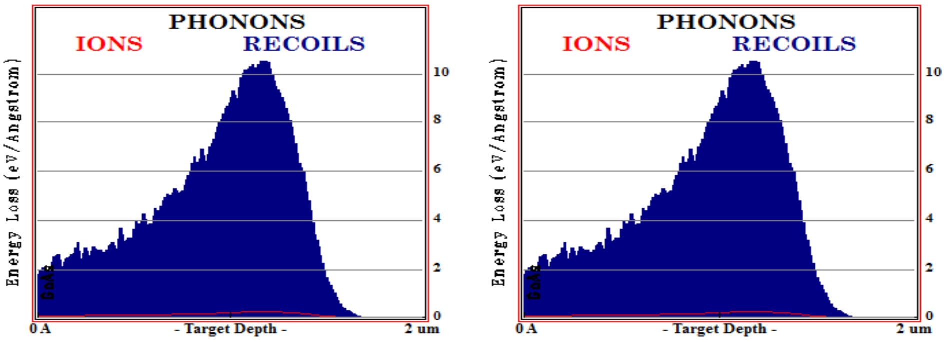


(a) (b)

Fig.4. Ions and recoils ionization curves for 1Mev O^{--} of: (a) GaAs, (b) Si.

3.5. Phonon production

Phonons are energy stored in atomic vibrations in a crystal. Since all the atoms in a crystal are linked, when you start vibrating one of them, then many of the other atoms start vibrating. This mass vibration is described as a phonon, since it is somewhat quantized (certain vibration modes are preferred). Fig. 6 illustrates the produced phonons, red line (in bottom) shows the ion loss energy transferred to phonon; we can note for both cases, that the energy loss coming from recoil to produce phonons is more higher than that which coming from oxygen ions.



(a) (b)

Fig.6.The distribution of target phonons produced in: (a) GaAs, (b) Si.

A summary of the energy loss is shown in Table 1 of 1 Mev oxygen implantation; the statistic indicate that, in the case of GaAs target the ions losing only a small amount of its energy 0.20%, to phonons, while the recoils are depositing 8.10 % of the energy into phonons. In the Si target, the ions losing 0.13%, while the recoils losing 5.94% of its energy. For two cases, we note that the energy loss to phonons production is less than that to ionization. Vacancy production amounts to few per cent of the total energy in two cases.

Table 1.Statistic for energy loss %.

Energy loss	Si		GaAs	
	Ions	Recoils	Ions	Recoils
Ionization	90.87	2,73	88.73	2.51
Vacancy	0.04	0,30	0.05	0.41
Phonon	0.13	5,94	0.20	0.81

4. Conclusions

Ion implantation simulation of oxygen ions in silicon (Si) and Gallium arsenide (GaAs) materials revealed that most of the energy loss is due to ionization and phonon production, in this latter most of energy loss is resultant of silicon and Gallium arsenide recoils. Vacancy production amounts to few per cent of the total energy.

The ions distribution and penetration depth was determined as well as understanding the formation of defects in GaAs and Si following oxygen implantation. The implanted ions have a concentration profile as a function of Gaussian-type depth; oxygen produced more vacancies and implanted deeper in Si compared to GaAs.

References

[1] S. Ahmed, P. Too, R. Gwilliam, B. J. Sealy, Appl. Phys. Lett.**79** (21), 19 (2001).
[2] M. Goorsky, Ion Implantation, Edited by Published by InTechJanezaTrdine **9**, 51000 Rijeka, Croatia Copyright © 2012 InTech.
[3] J.F.Gibbons; "Ion Implantation in Semiconductors", Proceedings of the IEEE; **66**, 9 (1972).
[4] A. L. Bloa, D. T. Quan, Z. Guennouni, P. N. Favennec, Revue Phys. App.**24**, (1989).
[5] K. Nordlund, J. Peltola, J. Nord, J. Keinonen, Journal of Applied Physics**90**, 4,(2001).
[6] G. Carter, W. A. Grant, Ion implantation of semiconductors, 1'1 ed. London: Edward, 1976.
[7] S. O. Kucheyer, J.S.Williams, C. Jagadish, L. Zou, G. Li, Phys. Rev.B**62**, 7510 (2000).
[8] A. Davies, Ion implantation and Beam proessing, edited by J. S.Williams and M. Poate, Sydney: Academic(1984).
[9] J. R. Srour, J. Marshall, Paul W. Marhal, IEEE Transactions on nuclear science **50**, 3(2003).
[10] F. Ziegler, P. Biersack, U. Littmark, Stopping Power and Ranges of Ions in Solids. New York: Pergamon, (1985).
[11] S. Martinie, T. S. Saoud, S. Moindjie, D. Munteanu, J.L. Autran, Nuclear Instruments and Methods in Physics Research B **322** (2014).
[12] J. P. Biersack, L. G. Haggmark,Nuclear Instrum. Meth Phvs. Res. B**174**, 1 (1980).
[13] W.O. Li, X. H. Xiao, A. L. Stepanov, Z. G. Dai, W .Wu, G. X. Cai, F. Ren, C. Z. Jiang, Li et al. licensee Springer, (2013).
[14] S.J.Pearton, Materials Science Reports 4 (1990).