MONTE CARLO SIMULATION OF NUCLEAR RADIATION EFFECTS IN NANOSCALE PHOTONIC MATERIALS

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ABSTRACT. *Study for penetration of nuclear radiation into semiconductor materials had been of theoretical interest and of practical important in these recent years, driven by the need to control material properties at nanoscale. Gallium Arsenide (GaAs) is a basic photonic material for most of the space technology communication, and, therefore, lends itself for applications where this is of concern. In this paper, the damage evolution due to Gamma (γ) rays is being simulated in nanoscale GaAs layer using SRIM (Stopping and Range of Ions in Matter). TRIM (The Range of Ions in Matter) calculation is also used to simulate the amount of nuclear energy deposited in the collisions and recoil events. Besides, we also compared the radiation tolerance between the conventional scale and nanoscale GaAs layer. From the findings, it is observed that most of the damage formed in the GaAs layer induced by the nuclear radiations is caused by the creation of Frenkel defect. This is due to energy transferred by the energetic ion or recoiling target to the lattice atom is higher than its displacement energy. However, when the GaAs layer is scaled down (nanoscaling), it is found that the GaAs layer can withstand higher radiation energy, in term of displacement damage. The total amount of disorder and the distribution in the depth are highly depending on the ion species and their energy.*

Keywords. nanoscale; Gallium Arsenide (GaAs); Frenkel defect.

INTRODUCTION

Devices based on III-V semiconductors and nanostructure are expected to be vital components of future Microsystems as the higher demand for better functionality, range of application and robustness persist. For instance, the integration of III-V based components could potentially broaden the utility of Microsystems to the expanding fields of high frequency communications along with a wide host of optoelectronic based technologies (Lemmerhirt, and Wise, 2006). An additional class of materials which can expand the functionality of Microsystems is nanomaterials. The uniqueness of these materials is their size dependent of electronic, magnetic and optical properties; in addition, they can be functionally integrated into existing III-V based devices.

The multi-functional nature of Microsystems may best be exploited by employing them in rigorous radiation environments, such as space, where a low power consumption, small volume, and superior functionality are required. However, the radiation that a device endured can alter or damage the normal functioning and resulting

in critical system failure. 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) (Wendler, 2009)

Studies of this ion-solid interaction can be done by introducing atoms into a solid substrate by bombardment of the solid with ions in the electron-volt (eV) to mega-electron-volt (MeV) energy range. The physical properties for a particular solid substrate are always sensitive to the presence of a trace amount of foreign atoms. Mechanical, electrical, optical, magnetic and superconducting properties are all affected and sometimes may even be dominated by the existence of such foreign atoms (Nastasi *et al.*, 2004).

Monte Carlo (MC) ion-solid simulation is a class of computational algorithms that relies on binary collision model which used repeated random sampling to compute their results. The Monte Carlo method shows a number of distinct advantages over analytical calculations. Monte Carlo approach shows more precise treatment of elastic scattering and it allows the determination of angular and energy distributions. The program TRIM is developed based on the Monte Carlo approach and describes multiple scattering of projectiles near the solid surface (Khalal-Kouache *et al.*, 2007). The results obtained acquired averaging over many simulated particle trajectories (Nastasi *et al.*, 2004).

GaAs is an III-V compound semiconductor with a combination of gallium (Ga) and Arsenic (As). Each Ga and As atom occupying sites on one of the two face-centered-cubic, fcc, which make up a zincblende lattice structure (Sze, 2001). Each As atom is shared with four Ga nearest atoms. On the other hands, each Ga has four As nearest atoms. The structure of GaAs is arranged in a tetrahedral structure.

GaAs is very insensitive to heat. The melting point of it is at 1513 K. The hardness of this material can be said as in moderate; between 4 to 5 on Mohn's scale. GaAs has a higher saturated electron velocity (order 7000 cm2/Vs) and electron mobility. This makes GaAs materials 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. 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 (Neamen, 2011). Nonetheless, these devices are known to present several failure modes associated with their operation in radiation environments. Thus, the understanding of the processes which leads to device failure is crucial in order to meet the radiation hardness requirements.

In this paper, the damage induced to GaAs by Co-particles at different thickness simulated by SRIM-TRIM software package will be discussed.

EXPERIMENTAL DETAILS

The SRIM-TRIM calculation is applicable in ion-solid interactions and has a number of distinct advantages over analytical calculations based on transport theory. SRIM-TRIM

is based on Monte-Carlo simulation which calculates the interaction of energetic ions with amorphous targets. The TRIM simulation can calculate the stopping and range of ions (10eV-2GeV/amu) into matter using statistical algorithms and averaging results of the ion-atom collisions.

The TRIM code is based on the binary collision approximation (Khalal-Kouache *et al.*, 2007) and helps to enumerate the range of ions in matter and the damage event in the target during the slowing-down process. All moving atoms are referred as ions and all target atoms are referred as atoms. This simulation can show the full animation of the penetrating process, the recoil cascades and also the mixing of target atoms. 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 target atoms utilized in the simulation, GaAs has a band gap energy of E_g = 1.42eV at room temperature with a density of 5.316 g/cm^3. In this research, the damage induced by Co ions on the GaAs layer depth = 50 nm, 80 nm, 100 nm and 200 nm is simulated. The energies for the incident ions are varying from 50 keV up to 2MeV. The number of incident ions for each simulation is 1000. From the simulation, 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 energy loss, *dE/dx* of Co-ion in GaAs can be divided into two parts: the energy transferred by the Co-ion to the GaAs electrons (called electronic stopping or inelastic energy loss) and to the GaAs nuclei (called nuclear stopping or elastic energy loss). The electronic stopping and nuclear stopping energy loss of Co-ion in GaAs at different energy level are as shown in Table 1.

Table 1: The Electronic Stopping and Nuclear Stopping Energy Loss of Co-ion in GaAs

Ion Energy (keV)	dE/dx Electron (keV/ μm)	dE/dx Nuclear (kev/ μm)
50.0	1.23E+02	1.18E+03
100.0	1.74E+02	1.18E+03
500.0	4.45E+02	8.23E+02
1000.0	7.34E+02	6.06E+02
2000.0	1.17E+03	4.13E+02
3000.0	1.62E+03	3.21E+02

The electron energy loss is due to the following mechanisms:

- Direct kinetic energy transfers to Si electrons which is mainly caused by the electron-electron collisions
- Excitation or ionization of target atoms,
- Excitation of band or conduction electrons,
- Excitation, ionization or electron capture of the projectile itself.

Nuclear stopping involve average energy loss which results from elastic collisions by the moving Co-ion with GaAs atoms. At Co-ion velocity, v_{Co} significantly lower than the Bohr velocity of the atomic electrons, $v_o = 2.188 \times 10^8 cm/s$ (Nastasi *et al.*, 2004), the Co-ion carries its electrons and tends to neutralize by electrons capture. The nuclear energy loss for the elastic collisions with the GaAs nuclei at these velocities will be dominated. However, as the v_{Co} is increased, the nuclear energy loss diminished. The electronics energy loss will therefore, become the main interaction.

Figure 1a and Figure 1b show the trajectories of Co-ion at E_{Co} = 50 keV and E_{Co} = 2 MeV with a layer depth of 80 nm. Figure 2a and Figure 2b, however, show the penetration path of Co-ion in GaAs at E_{Co} = 50 keV and 2 MeV respectively with a layer depth of 50nm. The red dot in the ion track represents the vacancy created by the incident Co-ion which means that an atom in the GaAs is displaced from its lattice site. The red dots show that the Co-ion creates damage constantly. The clusters of green dots, namely recoil cascade, are the vacancies caused by the recoiling GaAs atoms.

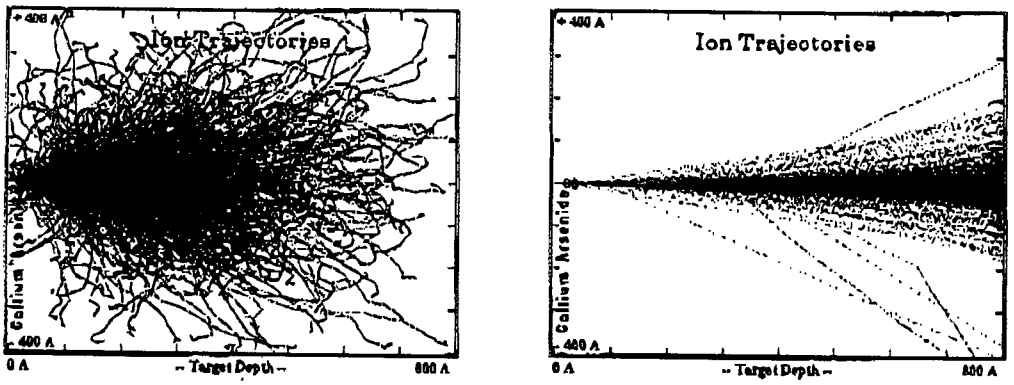

Figure 1. (a) The trajectories of Co-ion at E_{Co} = 50 keV (b) E_{Co} = 2 MeV

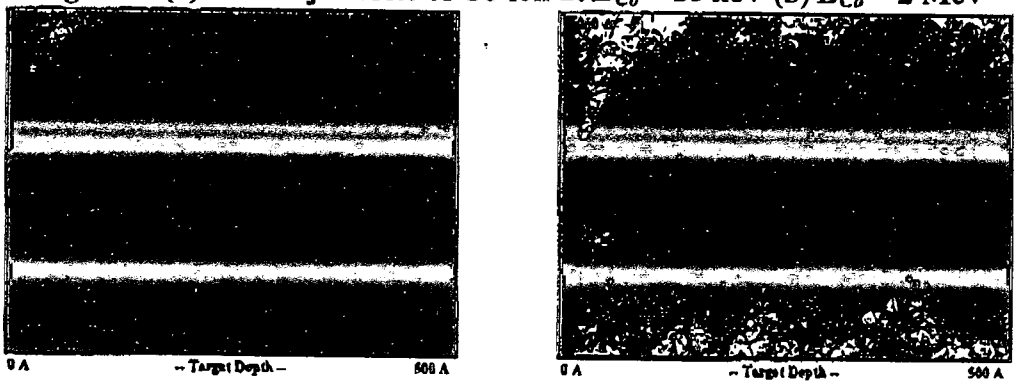

Figure 2. (a) The Co-ion track at Y-axis in GaAs at E_{Co} = 50 keV (b) E_{Co} = 2 MeV

When a Co-ion slows down and comes to rest in the GaAs, a number of collisions are made with the lattice atoms. In these collisions, lattice atoms which are displaced by the incident ions are known as primary knock-on atoms (PKAs). The energy required to displace the lattice atom represents the displacement threshold and is called the displacement energy, E_{disp}. The PKAs can in turn displace other atoms and ends up in creating a cascade of atomic collisions. This leads to the lattice disorder on the region around the ion track. The recoil energy, $E_{recoil} = E_{disp} - E_{latt}$ which is caused by the energy of E_{disp} will lost during the displacement of atom in its lattice position. Therefore, the value of E_{recoil} is higher than the value of E_{disp}. This will cause some vacancies in the lattice structure.

Figure 3a and Figure 3b show the number of target atom displacements per ion per Angstrom along the ion track at E_{Co} = 100 keV and E_{Co} = 1 MeV respectively. The highest curve shows the target displacements while the lower curve is the target vacancies. This indicates that there are fewer vacancies than the displacement in this collision event. The lowest curve shows the replacement collision which indicates the number of incident Co-ion that replaced the vacancy left by the recoiling GaAs atoms.

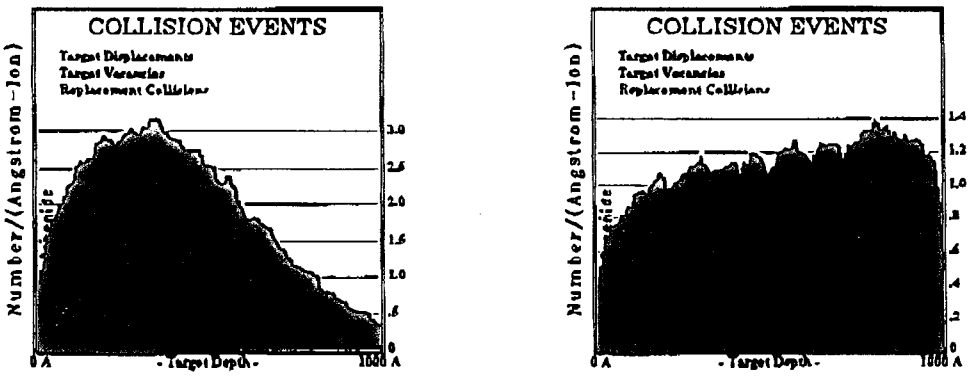

Figure 3. (a) The collision events in GaAs layer in GaAs at E_{Co} = 100 keV (b) E_{Co} = 1 MeV

The range R can be determined by the rate of energy loss along the path of the ion

$$R = \int_{E_{Co}}^{0} \frac{1}{dE/dx} dE \qquad \{1\}$$

R is defined as the total distance that the projectile travels in coming to rest. However, in most of the conditions and applications, the projected range, R_p, is the quantity of interest. R_p is the total path of length of the projectile measured along the direction of incidence where

$$R_p \cong \frac{R}{1+(M_2/3M_1)}. \qquad \{2\}$$

M_1 is the atomic mass of Co-ion (60 amu) and M_2 is the molecular weight of GaAs (144.63 amu) in this case. The projected range of Co-ion in energy range from 10keV to 3000keV is as shown in the plotting of Figure 4.

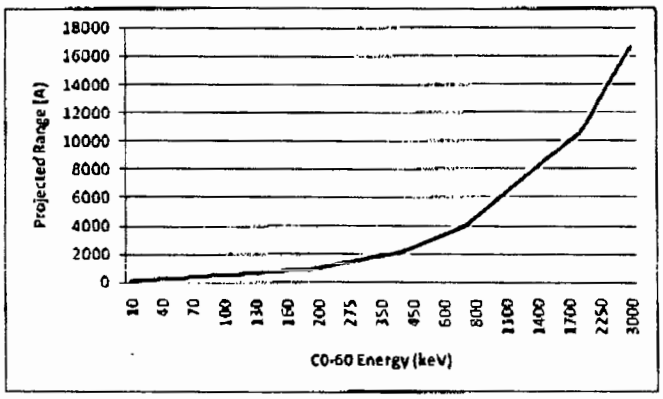

Figure 4. Projected range, R_p of Co-60 in GaAs.

Table 2, 3, 4, 5 and 6 show the range of the interaction of Co-ions with GaAs at E_{Co} = 50 keV, 100 keV, 500 keV, 1 MeV and 2 MeV respectively at different target depth. It is found that if the thickness of the GaAs target is small compared to the projected range (Fig. 7) at that particular E_{Co}, the energy loss in the target GaAs will be small. Therefore, when the depth of target is reduced, the range of damage is also diminished. Comparing the damage events and the energy absorbed by GaAs due to the deposition of Co-ion, it is observed that the damage density goes lower even at higher E_{Co}. This is due to the higher E_{Co} has higher projected range, thus, has less interaction with target.

Table 2: Range of the Interaction of 50 kev Co-ions with Gallium Arsenide (GaAs) obtained from the aimulation using TRIM.

Target Depth (nm)	Total vacancies	Replacement collisions	Energy Absorbed by GaAs (keV/ion)
50	964	25	43.60
80	1018	27	45.50
100	1019	27	45.50
200	1019	27	45.50

Table 3: Range of the Interaction of 100 kev Co-ions with Gallium Arsenide (GaAs) obtained from the simulation using TRIM.

Target Depth (nm)	Total vacancies	Replacement collisions	Energy Absorbed by GaAs (keV/ion)
50	1265	33	62.60
80	1829	48	84.50
100	1907	50	86.80
200	1973	52	89.30

Table 4: Range of the Interaction of 500 kev Co-ions with Gallium Arsenide (GaAs) obtained from the simulation using TRIM.

Target Depth (nm)	Total vacancies	Replacement collisions	Energy Absorbed by GaAs (keV/ion)
50	621	16	43.80
80	1207	32	76.50
100	1740	46	100.00
200	3984	105	203.0

Table 5: Range of the Interaction of 1 Mev Co-ions with Gallium Arsenide (GaAs) obtained from the simulation using TRIM.

Target Depth (nm)	Total vacancies	Replacement collisions	Energy Absorbed by GaAs (keV/ion)
50	414	11	32.50
80	783	21	52.70
100	1085	28	71.60
200	2452	65	139.60

Table 6: Range of the Interaction of 2 Mev Co-ions with Gallium Arsenide (GaAs) obtained from the simulation using TRIM.

Target Depth (nm)	Total vacancies	Replacement collisions	Energy Absorbed by GaAs (keV/ion)
50	272	7	21.90
80	526	14	38.80
100	685	18	49.40
200	1424	38	87.30

CONCLUSIONAND FUTURE WORK

From the simulation, Co-ion is shown to impose dislocations and other types of electrical active defects in the GaAs layer. The degradation in the GaAs materials is found highly relying on the projected range of the Co-60 ions. Therefore, down scaling the GaAs layer shows improved radiation robustness against the Co-60 radiation. However, the other factors such as quantum size effect, the energy gap between the

conduction and valence band and etc. must also be taken into consideration when the dimension of the device is diminished.

In future, the examination of radiation effect on nano-scale devices using real test monitoring would be studied. This is because there is a current need for small-scale power supplies which can be used to power microsystems thereby enabling autonomous functionalities. The future use of nano-satellites will also prompt the implementation of state-of-the-art microelectronic components and systems.

ACKNOWLEDGEMENTS

The authors are thankful to Science Fund 2007, MOSTI, Project No.: SCF0046-STS-2007, with title "Effects of Total Dose Irradiation on Semiconductor Devices".

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