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6. Estimation of neutron irradiation damages in Ni/n-GaAs Schottky contact layers via FLUKA Monte Carlo simulations

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Abstract. We estimated radiation effects of Ni/n-GaAs contact Schottky in neutron field by FLUKA Monte Carlo Code. Firstly, we determined elemental ingredients and layer thicknesses of diode by WDXRF spectroscopy technique. Then irradiation process was simulated in 1MeV neutron field for Ni/n-GaAs Schottky contact by FLUKA code. Results were interpreted for the purposes of Schottky diodes used in radiation applications.

Introduction

Because of its successful electronic applications, Schottky contacts are used in a large field. It is an important issue that how Schottky diodes are affected by application conditions. Radiation application of Schottky contacts is a popular research field [1- 5].

FLUKA is able to simulate interactions and transports of many particles as hadrons, heavy ions and electromagnetic particles in a large perspective from

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few keV (or thermal neutron) to high cosmic ray energies. The useful modern physics methods used in the development of the code have enhanced the usefulness of the code in different areas [6]. It is possible to predict lots of quantities from residual dose rates to activity of long-lived radionuclides by using FLUKA with an excellent accuracy [7]. Agosteo et al., studied direct interactions by irradiating a commercial PIN diode with thermal and fast neutron fields and compared experimental and FLUKA simulations for their solid state microdosimeter studies. Their study show that the consistency of the simulation results with the experimental data is satisfactory if the approximation made for the detector geometry is taken into account [8]. Neutron spectrometry was investigated with a recoil radiator-silicon detector device in another research. In the study the spectra of deposited energy were also calculated analytically via Monte Carlo simulations by FLUKA code. The effect of secondary charged particles produced by thermal and fast neutron interactions in the silicon diode was also investigated. FLUKA simulation of the deposited energies in the silicon diode for 2:7 MeV energetic neutrons and the results were compared to the experimental and analytical curves [9]. Wind investigated the energy response of RADFET for a wide spectrum of subatomic particles and photons from high energy photons, electrons and protons to neutrons by using FLUKA code [10]. Butterworth et al., estimated the radiation damage in the LHC cavities arising from beam gas collisions by FLUKA [11]. Korkut et al. recommended a new radiation shielding material by using FLUKA code [12].

Changing in electrical characteristics was studied depending on radiation effects on Schottky contacts in most studies. Interface spesific region has an effective role in the performance of Schottky contacts [13]. The change in Schottky diode characteristics depending on radiation environment is usually attributed to possible changes in metal-semiconductor interface region. But the origin of radiation effects in Schottky diode is not known in all its bearings. We used FLUKA simulation tool to see interactions in Schottky contact layers in the effect of 1 MeV energetic neutrons. In this stage the interaction of neutron irradiation with Ni/n-GaAs Schottky contact is discussed with respect to (dpa) displacements per atom and absorbed doses.

Experimental details

In this paper, we used n-type GaAs wafer (Si-doped), (100) oriented with the free carrier concentration of $7.3\text{x}10^{15}$ cm^{-3} at room temperature conditions. In the chemical cleaning process the wafer was cleaned in trichloroethylene, acetone, and methanol for 3 minutes. After the chemical cleaning process, to remove the surface damages and undesirable impurities wafer was etched with

H_2SO_4:H_2O_2:H_2O (5:1:1) for 1 minutes [14, 15]. For the fabricating of ohmic contact, a very small piece of indium was evaporated on the back side of the n-GaAs wafer and then the structure was annealed at 300^0C for 3 minutes in N_2 atmosphere to get low resistant ohmic contact. Ni evaporation was applied on the front face of the n-GaAs wafer as dots to get high quality Schottky contacts with the diameter of about 1.0 mm. Schottky contact layers are formed as seen in Fig.1. A wavelength-dispersive X-ray spectrometer (WDXRF, Rigaku ZSX-100e with Rhodium target X-Ray) was used to obtain elemental contents of diode. The sensitivity of WDXRF measurements is about ppm. As seen in Table.1, contents of diode were used in simulation process [16].

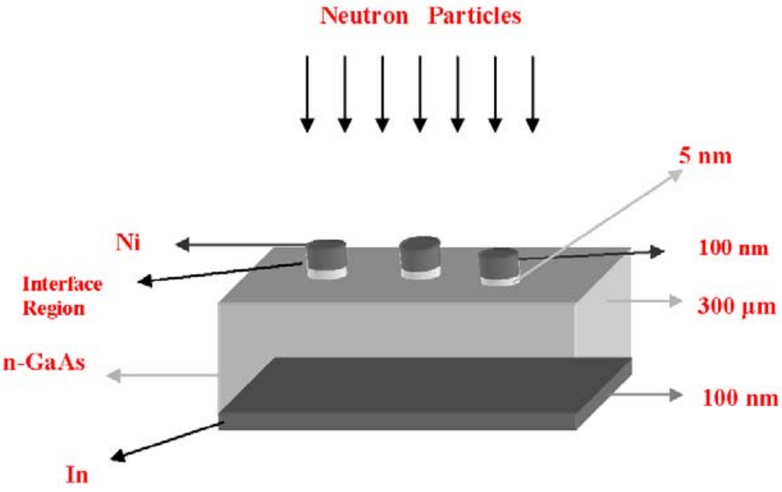

Figure 1. Layers and layer thicknesses of Ni/n-GaAs Schottky diode used in simulation process.

Table 1. % Contents of Ni / n-GaAs Schottky Diode obtained from WDXRF results.

Contents of Diode	***% Weight***	**Uncertainty**
Element	Referenced Sample	
Ga	49,257	±0.000049257
As	48,500	±0.000048500
O	1,793	±0.000001793
Ni	0,438	±0.000000438
Si	0,012	±0.000000012
Compounds with Oxygen		
Ga_2O_3	51,068	±0.000051068
As_2O_3	48,474	±0.000048474
NiO	0,437	±0.000000437
SiO_2	0,020	±0.000000020

Simulation process

Firstly thicknesses, densities and elemental contents (obtained from WDXRF measurements) of Schottky contact layers were entered FLUKA input file for primary 1 MeV neutron energies. Then simulation geometry has formed as seen in Fig 2. In this diagram Ni/ *n*-GaAs/In Schottky diode is in the center of simulation geometry. The Schottky contact is exposed to 1MeV neutrons along z axis. Schottky contact layers and their thicknesses are seen in Fig.1. As seen in Fig. 1, regions are labeled as below.

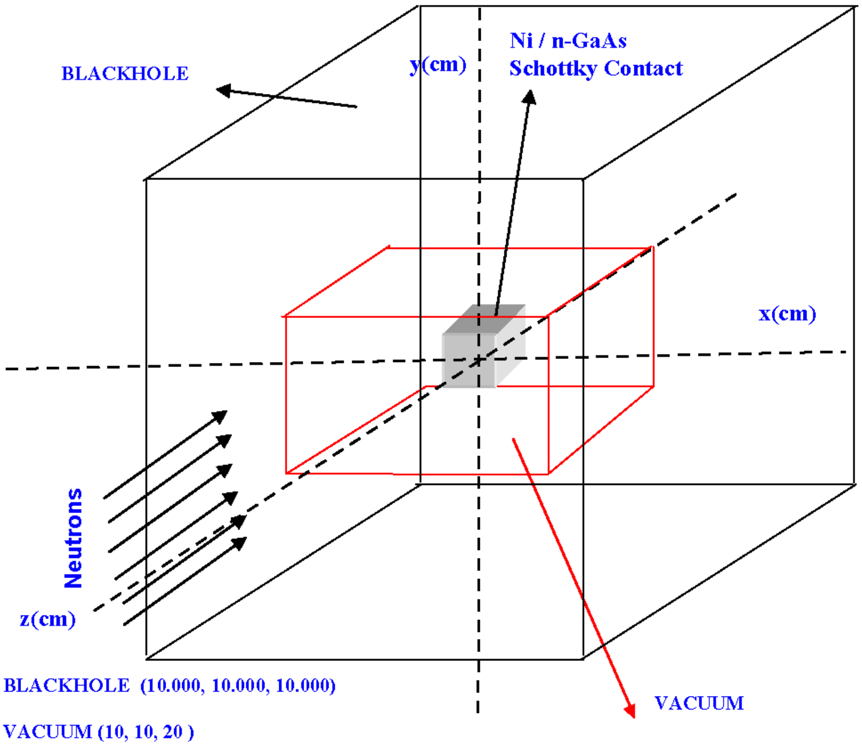

Figure 2. Simulation geometry of neutron irradiation processes in Ni/n-GaAs Schottky diode.

R1: Region 1; Black hole
R2: Region 2; Vacuum
R3: Region 3; Nickel, Schottky Metal Layer
R4: Region 4; (Ni / *n*-GaAs), Interface Layer
R5: Region 5; *n*-GaAs (Si Doped), Semiconductor Layer
R6: Region 6; Indium, Ohmic Contact Metal Layer
R7: Region 7; Vacuum

We used NEW-DEFAults card to active some settings about simulation conditions (Inelastic form factor adjustments to Compton scattering were activated. Particle transport and production threshold arrange as 10 MeV. Multiple scattering thresholds lowered to 20 MeV for secondary charged particles. Heavy particle bremsstrahlung activated with indicates photon production above 1 MeV- *http://www.fluka.org/fluka.php?id=man_onl*). USRBIN estimators were located the exits of each layers to calculate absorbed radiation doses and dpa values for each region. The program was run for 10^6 primaries for each irradiation processes. Dose values in each region (GeV/g/pr) are read in FLUKA output files. Uncertainties in simulation results are approximately %1.

Results and discussion

Contact materials have precious place in the quality of Schottky contacts. Electrical conductivity of contact metal, carrier concrentation and band gap of semiconductor is impressive factors for electrical conduction mechanisms in Schottky diodes. Fabrication processes affect the chemical and physical properties of contacts as surface roughnesses and metal semiconductor interface transformations. The properties of surface and interface are directly interested in chemical cleaning and vacuum coating conditions. In this procedure, there are always been inadvertent effects. The all above reasons affect chemical ingredient rates and electrical dipole transformations of Schottky diodes. We assumed that these effects were in a minimum level in simulation process. Ni/ *n*-GaAs Schottky diode includes nickel as Schottky contact metal; indium as ohmic contact metal. n-type GaAs substrate is composed of gallium, arsenic and silicon. According to WDXRF results, there are four oxygenate compounds in interface oxide layer: Ga_2O_3, As_2O_3, NiO and SiO_2 as shown in Table 1. We used the compositions, thicknesses and densities of Schottky contact layers in simulation process. WDXRF measurement sensitivity can affect the results of simulations. Small differences in content measurements may cause small differences in simulation results. Interface layer properties of Schottky contacts have an unneglectable importance in terms of conduction mechanism [13].

Fast neutrons produce a modification of the lattice structure and they affect the mechanical, electrical and other physical properties of irradiated materials. The incident particle kinetic energy may be transferred to the target atom in collision process. If the energy gets over a given transference threshold limit value, the target atom is displaced and then a stable vacancy pair and interstitial location (called Frankel pair) is created [18]. Neutrons cause non-ionizing effects in irradiated materials. Nonionizing energy can disturb the periodicity of the crystal. So, new deep states and trapping center formations are created into the material. The states can be changed by band gap of the material [19]. If irradiated material is an electronic structure including transistors or diodes, all the components which compose the structure must be taken into consideration. Metals, basic semiconductor bulks, interface oxide regions, organic components *etc*. are keystones of electronic curcuit technology. Schottky diode, one of the most important elements of modern electronic world, is usually a multi-layered structure. Our sample (Ni/n-GaAs Schottky diode) has metal, semiconductor and interface oxide regions. We simulated 1 MeV neutron irradiation process for our sample. According to the simulation results, the interface layer absorbed maximum radiation doses as compared to the other layers. Absorbed doses by the each layer were shown in Fig.3. Dpa (displacements per atom) is a measure for damage amount for irradiated materials. Displacement damage can be produced by all the particles. There is a direct relation between the dpa value and the total numbers of defects (or Frenkel pairs). When *x* atom in the material has been displaced from its position, *x* quantitiy of dpa has been located in the lattice of the material [17]. Maximum absorbed doses caused the maximum quantity of dpa in interface layer as can be seen in Fig.3 and Fig.4 by the reason of 1 MeV energetic neutron irradiation. And so new interface dipole transformations were located in the interface layer. This result is consistent with experimental results and Tung's theory [1, 13]. Akkurt *et al.*, irradiated their Schottky diode with neutrons. They observed that electrical characteristics of diode changed with the effect of neutron field. Radiation damages were not only located in the interface layer, but also in the other layers as can be seen in Fig.4. There was a characteristic change in all the layers of electronic structure of Ni/n-GaAs Schottky diode due to neutron irradiation.

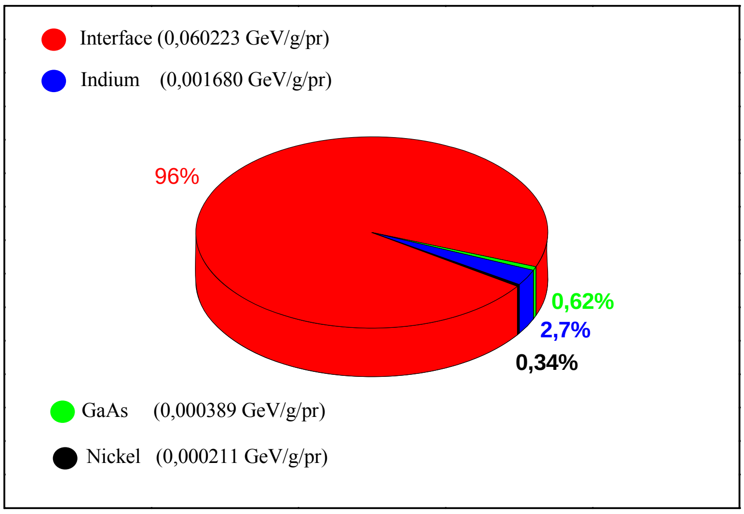

Figure 3. Absorbed doses for neutron irradiation by layers of Schottky diode.

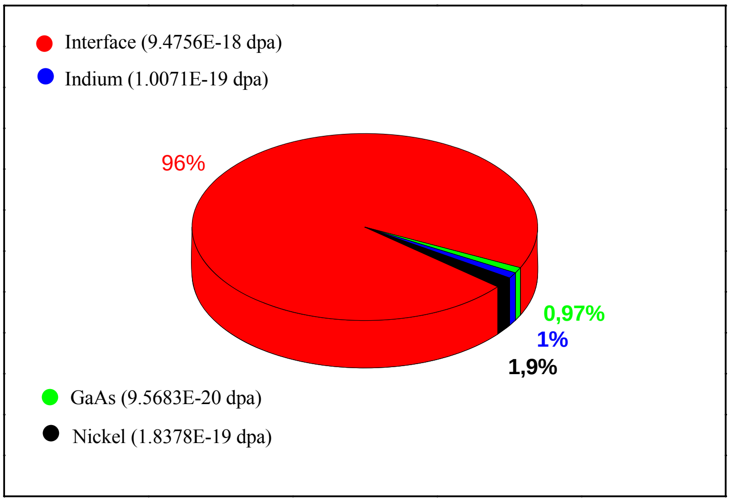

Figure 4. Dpa values for neutron irradiation by layers of Schottky diode.

Conclusion

We fabricated Ni/n-GaAs Schottky contact in the form of Fig.1 and determined its elemental contents by WDXRF. FLUKA Monte Carlo Code was used to simulate 1 MeV energetic neutron irradiation process. Neutron field effect of dpa (displacements per atom) quantities and absorbed doses of the Ni/n-GaAs Schotttky contact layers were calculated by FLUKA for 1 MeV energetic neutrons. By way of addition, the implicit role of interface region in radiation field was emphasized via its maximum dose absorbtion and maximum dpa quantity property. These results enable us a foresight on neutron field induced electrical dipole changes in the interface layers. As a result, FLUKA simulations provide more efficient properties for Schottky contacts in different radiation conditions. To be able to estimate radiation effects on materials give us a proper way for choosing contact materials in the optional radiation applications. So, possible negative effects can be minimized under different radiation conditions.

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