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Characterization of New Structure for Silicon Carbide X-Ray Detector by Method Monte Carlo

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This work presents a characterization of radiation absorption properties of silicon carbide (SiC) as semiconductor for the realization of detectors for X-rays. SiC detectors can potentially reach superior performance with respect to all the other semiconductors presently employed in hazardous environments in nuclear and space science and technology. Physics and numerical modeling of photons transport through SiC detector is incorporated in non-destructive Monte Carlo method for determining the energy deposited and dose distribution. The Monte Carlo code has been adopted for numerical simulations for different detector conditions and configurations. The X-ray characterization of new SiC structures originates the improving of design of these detector systems.

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1. Introduction

Silicon carbide (SiC) research has diversified enormously in recent years from its "traditional" base in power switching diodes into a wide range of applications such as trace gas sensing, UV detection, neutron counting, particle tracking, alpha particle detectors, X-ray analysis, and light ion detection. Also, after exposure the SiC Schottky diodes to 50 MeV proton fluxes of 10^{13} cm^{-2} it is appointed that useful spectroscopic operation even maintained [1].

New detectors based on this wide bandgap semiconductor (E_g = 3.26 eV) could also find applications in areas such as biosensors and small imaging as well as environmental monitoring. Future space investigation will also require detectors to operate in harsh radiation environments and in wide range of temperature. In Ref. [2] described first experiments for characterization of a radiation-hard X-ray spectrometer capable of operation at high temperatures which matches the mission aims of European Space Agency. The need for high-efficiency low-energy spectroscopy was the driving force behind the development of a new ultra-thin Schottky contact. The ultra-thin Schottky contact ($\cong$ 18 nm Ni/Ti) minimizes the absorption in the electrode structure resulting in higher efficiencies (up to 100 times) for low-energy X-rays ($<$ 10 keV) compared to standard Schottky diode contact, where Ni or Ti (contact thickness $>$ 100 nm). Hence, semi-transparent SiC Schottky diode (STSSD) is name of new X-ray detector.

A Monte Carlo model has been developed to predict the X-ray spectroscopic performance of silicon carbide detectors over range 1 keV–60 keV [3]. This MC model has adequate great vacancy for improvement in determination of energy resolution.

Owing to the problems recognized in practice, the aim of our paper is to determine the energy deposited in a 4H-SiC wafer of detector using computer simulation based on the Monte Carlo techniques. Advanced computer program FOTELP-2K10 [4] was used for this purpose. The obtained results provided conclusions regarding the possibilities of applied codes in analyzing semiconductor characteristics in radiation fields.

2. Theory

The energy resolution of detector is usually given in terms of the full width at half maximum of the peak (FWHM) [5, 6]. In general, the energy resolution is a function of the energy deposited in the detector. This is due to the Poisson or Poisson-like statistics of ionization and excitation. It is found that the average energy required to produce ionization is a fixed number w, dependent only on the material.

Thus as deposited energy E_d increases, the number of the ionization events also increases resulting in smaller relative fluctuations. If the full energy of the radiation is absorbed as is the case for detectors used in spectroscopic experiments, the energy dependence of the resolution is:

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$$R = g \cdot \sqrt{\frac{F \cdot w}{E_d}}, \tag{1}$$

where g is the factor 2.35 relates the standard deviation of Gaussian to its FWHM. F is a number known as the Fano factor that is function of all the various fundamental processes which can lead to an energy transfer in the detector. This includes all reactions which do not lead to ionization as well, for example, phonon excitations. It is thus an intrinsic constant of detecting medium. This contributes greatly to enhancing the resolution of semiconductors which already profit greatly from the small average energy (w) to create an electron-hole pair. For silicon, the energy to create an electron-hole pair is determined experimentally and amounts 3.73 eV [7] and for 4H-SiC is 5.05 eV [8]. A measurement of the mean Fano factor for the pair number distribution is almost constant with small fluctuations around the value of 0.117 [9].

In a SiC Schottky power diode, the thermionic emission process dominates in the transport of current across a metal n-type semiconductor contact [10]. Under forward bias condition, the current flow across the Schottky barrier is given by:

$$I = r \cdot T^2 \cdot \exp\left[\left(\frac{qV_D}{\Theta kT}\right) - 1\right] \cdot \exp\left(-\frac{q\Phi_B}{\Theta kT}\right) \tag{2}$$

where Φ_B is the barrier height between the metal and n-type semiconductor, T is the absolute temperature, q is the charge of an electron, k is the Boltzmann constant, $\mathit{\Theta}$ is ideal factor, r is the Richardson constant, V_D is the voltage drop at the Schottky contact. For 4H-SiC the theoretical value of the Richardson constant is 146 A $\mathrm{cm}^{-2}\mathrm{K}^{-2}$. The ideal factor $\mathit{\Theta}$ can be derived from a voltage-current (V-I) characteristic curve and he depends of energy deposited E_d.

3. Characterization method

3.1 Geometry and Materials

In order to use numerical methods in this paper, the appropriate geometry form of the SiC detector [2, 3] was defined using adequate software. FOTELP program uses RFG geometry [11] for detector geometry description. According to the available manufacturer data for a new SiC detector, semi-transparent 4H-SiC Schottky diodes were fabricated from wafers produced that have 20 μm epitaxial layer grown on a 370 μm substrate (Fig. 1). A Cr/Ni based ohmic contact was deposited on the rear face of the substrate. Thereat, silicium oxide that has a 25 nm thick was grown to passivate the surface. Figure 1 shows a scheme of the diode cross-section, detailing the layers and structures, with their thicknesses. The size of diode's base was 180 × 180 $\mu\mathrm{m}^2$.

3.2 Numerical method

Characterization of X-ray SiC detector STSSD by Monte Carlo method made with FOTELP-2K10 code. FOTELP-2K10 code has great competency in successful resolving of radiation transport problems which review interactions gamma and X-rays with electronic components and devices, such as MOSFET dosimeters [12, 13], CdZnTe detector [14] and diamond detector [15].

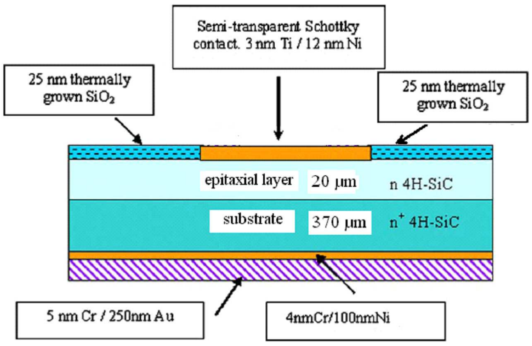

Fig. 1. Cross-section of SiC detector STSSD (layers not to scale).

Physical rigor is maximized by employing the best available cross sections and high speed routines for random values sampling from their distributions, and the most complete physical model for describing the transport and production of the photon/electron/positron cascade from 100.0 MeV down to 1.0 keV. FOTELP-2K10 is developed for numerical experiments by Monte Carlo techniques for dosimetry, radiation damage, radiation therapy and other actual applications of these particles. For the photon history, the trajectory is generated by following it from scattering to scattering using corresponding inverse distribution between collision, types of target, types of collisions, types of secondaries, their energy and scattering angles. Photon interactions are coherent scattering, incoherent scattering, photoelectric absorption and pair production. Doppler broadening in Compton scattering are taken. The histories of secondary photons include bremsstrahlung and positron-electron annihilation radiation. The condensed history Monte Carlo method is used for the electron and positron transport simulation. During a history the particles lose energy in collisions, and the secondary particles are generated on the step according to the probabilities for their occurrence. Electron (positron) energy loss is through inelastic electron-electron (e^-,e^-) and positron-electron (e^+,e^-) collisions and bremsstrahlung generation. The fluctuation of energy loss (straggling) is included according to the Landau's or Blunk-Westphal distributions with 9 gaussians. The secondary electrons, which follow history of particles, include knock-on, pair production, Compton and photoelectric electrons. The secondary positrons, which follow pair production, are included, too. With atomic data, the electron and positron Monte Carlo simulation is broadened to treat atomic ion relaxation after photo-effect and impact ionization. Flexibility of the codes permits them to be tailored to specific applications and allows the capabilities of the codes to be extended to more complex applications, especially in radiotherapy in voxelized geometry using CT data.

The actual version of FOTELP-2K10 [4] program was expanded by adding new routines for accepting from XCOM [16] data for photon interaction, adapted routines for coherent and incoherent scattering and annihilation, and new PENGEOM6 package for geometry modeling. In this way, Monte Carlo simulations were being improved, particularly at low energies that are typical for simulations in dosimetry and radiology.

4. Results and discussion

The general scheme of physical model used in Monte Carlo simulation described in Sec. 3. is applied to the specific geometrical configuration represented in Fig. 1 and for various material layers arrangements. In numerical experiment monoenergetic beam of photons containing 10^7 particles is incoming perpendicularly to the upper surface of the sensitive volume. Photon's energies were 10 keV, 18 keV, 26 keV, 60 keV and 100 keV. The absorption of X-rays as a function of X-ray energy can be calculated using well-known methods [5, 16].

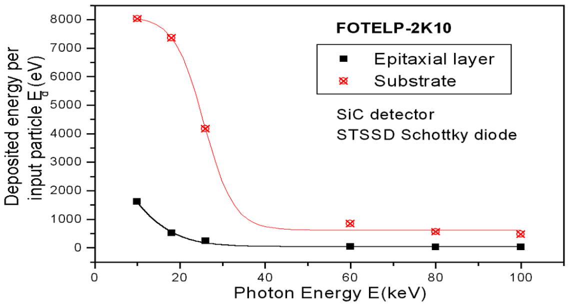

Fig. 2. Deposited energy vs. photon energy for epitaxial layer and substrate. Calculation with FOTELP-2K10 code for SiC detector (STSSD Schottky diode).

Calculation values of deposited energy in epitaxial layer and substrate are presented at Fig. 2. Functional dependence $E_d(E)$ is fitting with Boltzmann equation:

$$E_d = \frac{E_1 - E_2}{1 + \exp(\frac{E - E_0}{\Delta E})} + E_2 \tag{3}$$

Where, the $E_d(E_0)$ value at photon energy $E = E_0$ is half way between the two limiting values for photon energy range of interest, E_1 as a initial value and E_2 as a final value. The width of energy range is approximately ΔE, and E_0 is center of a range of the photon energy. Fitting parameters for calculation of deposited energy per input particle in two material zones are presented in Table.

All trajectories of the particles within the structural components of detector were monitored to register deposited energy in material zones and total number of ionizations per input particle. Total deposited photon energies in the detector material zones (epitaxial wafer and substrate) are shown in Fig. 2.

The most interesting zone in our case is the epitaxial layer. From Fig. 2 one can see that in this zone the efficiency of detection decreases with increase of X- ray energy within low X-ray energy range from 10 keV to 100 keV. This fact may cause additional difficulties in detector signal processing if the corresponding electronically system and must necessarily be taken into account.

TABLE

Fitting parameters for calculation of deposited energy per input particle

Material zone	E_1 (eV)	E_2 (eV)	E_0 (keV)	ΔE (keV)
Epitaxial layer	4570.95	38.35	6.36	5.67
Substrate	8115.22	625.58	25.62	3.49

One of radiation transport characteristics is dependence for number of ionization in function of photon energy, which is shown in Fig. 3.

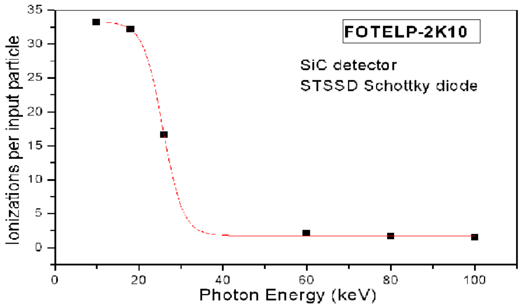

Fig. 3. Number of ionizations vs. photon energy, calculation with FOTELP-2K10 code for SiC detector (STSSD Schottky diode).

Inspecting the Fig. 3 one can see that the number of ionizations decreases with increase of X- ray energy according relation:

$$J = \frac{J_1 - J_2}{1 + \exp(\frac{E - E_{J0}}{\Delta E_J})} \tag{4}$$

Where are: $J_1 = 33.23$, $J_2 = 1.73$, $E_{J0} = 25.73$ keV and $\Delta E_J = 2.33$ keV.

5. Conclusion

In this paper, numerical experiments for characterization of energy resolution in function of deposited energy, which is important parameter for SiC detector STSSD, are demonstrated. The results obtained can help one to choose such materials which are of interest for a more detailed experimental investigation. In fact, for each special type of SiC detector one can perform Monte Carlo simulation before experimental investigation in X-ray fields in order to obtain in advance sufficiently reliable information about the expected response of the detector with a defined structure. In this way one can choose such a structure which has optimal response for a defined range of energy. Our intention in this paper was, among other things, to initiate ideas on how to set up appropriate experiments, which would follow conditions imposed on numerical simulations. However, the problem of electrical measurements of properties in medium that has microscopic (or even less) dimensions are well known. Thus, the purpose of this paper is to present the possibilities of the numerical simulations for the deposited energy distribution on microscopic, submicroscopic and supernanoscopic levels, primarily in qualitative sense. Predicting the performance characteristics of detectors can reduce development costs and help to design systems closely matched to the application and operating environments. Further investigations in other areas of interest, related to the study of electrical and technological characteristics of components necessary in the silicon carbide (SiC) and related material physics, are planned.

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