MCNPX CALCULATIONS FOR ELECTRON IRRADIATED SEMICONDUCTOR DETECTORS

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1. Introduction

Electron-beam irradiation represents a very effective tool for modification of material properties in a well-controlled way. In physics research, radiation processing can be used for two main purposes: a) as a technological tool for intentional and custom-tailored control of material properties of interest [1, 2], but also b) as a tool for studying damage, aging and degradation of materials under exposure to radiation [3, 4].

The process of irradiation is a complex task comprising precise setting of many parameters concerning the accelerator itself and the irradiation geometry. In order to obtain required characteristics of the studied material, the exact knowledge of the incident beam parameters and in many cases also quantification of processes in an irradiated material are needed. Here, the simulation of the electron beam transport using a computer code proved as very useful. We would like to show how the Monte-Carlo approach based transport code MCNPX (Monte Carlo N-particle eXtended) can be used to contribute to a deeper understanding of electron interaction processes in semiconductor structures and to solve some practical problems of electron beam irradiation. The modelled geometry corresponds with the arrangement of the semiconductor detectors irradiation carried by the electron accelerator UELR 5-1S (The University Centre of Electron Accelerators at the Slovak Medical University), designed for radiation treatment in routine production and in research.

2. Electron transport by MCNPX code

MCNPX is a widely spread calculation code based on Monte Carlo algorithms used to simulate interaction of radiation with matter. It contains high-quality physics and has access to the most up-to-date cross-section data. The newer MCNPX version 2.7.0 enables to follow the transport of 34 particle types at nearly all energies. Therefore, its applicability has been considerably extended, mainly in the field of material research.

As an electron travels through a medium, it interacts continuously with the electrons through the long-range Coulomb force. Thus, the interactions between an electron and the medium are much more frequent than those of neutral particles. An electron typically undergoes roughly 10^4 more collisions for the same energy loss than a neutral particle. Therefore, the simulation event by event would not be convenient and the electron transport in MCNPX is carried out using condensed history algorithm. In a condensed history, several scatterings of an electron are approximated by a single event using multiple scattering theories. The outcome of the multiple scatter is assumed to be the accumulation of individual scatterings [5].

3. Materials and Method

The model geometry used in the simulations comprised a box representing the detector filled with a semiconductor material (GaAs, SiC or Si). The box (4×4 mm in size, 270 μm thick) was placed on an iron board with a thickness of 0.5 cm and a size of 40×5 cm. The electron beam was modelled as a disk source with a diameter of 2 cm emitting monoenergetic 4 or 5 MeV-electrons monodirectionally toward the detector. The distance between the foil of the accelerator exit window and the iron board was about 54 cm; the outside medium was air. 10^6 source particles (s.p.) were simulated each time. All calculations were carried out in coupled electron-photon mode (MODE P E).

As first, the MCNPX simulations were used to study the flux densities of electrons (electron spectra) and deposited energies in three different semiconductor materials (GaAs, SiC an Si) for the electron beam energies of 4 and 5 MeV. Further, the relationship between the absorbed dose and the electron fluency was investigated. Although the experimental equipment of the irradiation facility allows determining the dose absorbed in an irradiated object, other laboratories may use the fluency to describe their experiments. For practicable comparison of the results obtained by different laboratories, the relation between these two quantities has to be known. In the case of very thin objects (like studied detectors [3]), the high energy electrons leave only a part of their energy in the material, therefore the conversion between the dose and the fluency is not simple and simulation is very helpful. Finally, to optimize the irradiation process and also the samples arrangement, knowledge of the dose depth distribution in an irradiated object is valuable. Hence, the dose depth profiles of detector materials irradiated by 4 and 5 MeV-electron beams up to the depth of 1.0 cm were calculated and additionally, the effect of backscattering from the iron board was followed. The dose depth distribution in GaAs irradiated by 4 MeV electrons was compared with the experimentally obtained values of absorbed dose under 70 min irradiation [6].

4. Results and Discussion

MCNPX simulation showed that the dominant physical events contributing to electron creation during electron beam transport through a detector structure are similar for all investigated materials and they are as follows: knock-on (440 e^- per s.p.), electron Auger (7 e^- per s.p.), photo-electric (5 e^- per s.p.), Compton recoil (0.6 e^- per s.p.), photon Auger (0.3 e^- per s.p.) and finally pair production (0.002 e^- per s.p.). The mean energy of knock-on electrons is about 2.3 MeV and the electrons created by the other events have the mean energy between 1 and 80 keV. Totally about 460 electrons were created per source particle. Some of the electrons passed through the detector, while a part of them stopped due to the interaction processes. The energy spectra of electrons were scored on the top and back side of the detector using F2 tally subdivided into 300 energy bins. The scoring area was 0.16 cm^2. The energy spectrum (flux density divided into energy bins) of electrons scoring on the top surface and on the back side surface of the GaAs, SiC and Si detectors (after passing the 270 μm thick detector) are shown in Fig. 1. The spectrum from the top side shows that the initially monoenergetic electron beam (4 and 5 MeV) is distributed in energy after passing through a 54 cm thick air region and the position of the maximal energy is shifted to approximately 3.9 and 4.9 MeV, respectively. From the back side spectra it is obvious, that for a 270 μm thick detector, the amount of electron creation events dominates to electron losses (the range of 5 MeV electrons in GaAs, SiC and Si is about 5, 12 and 12 mm, respectively). On the back side spectra, hills from secondary knock-on electrons can be recognized. Their position changes according to the ionization potential of the detector material.

The energy deposited in a cell representing a detector was scored by means of F6 tally providing results in units MeV/g per s.p.. The obtained values were recalculated to desired dose rate units, Gy/s and are presented in Tab. 1 for GaAs, SiC and Si materials for 2 different energies of the incident electron beam, i.e. 4 and 5 MeV. The corresponding electron flux densities (given in $cm^{-2}s^{-1}$) were determined using F2 tally for electrons scored on the top of the detector (flux averaged over a surface), which are also listed in Tab. 1. To match the results from simulation with the experimental values of the absorbed dose, the source emissivity (electrons released per second) and the time of irradiation have to be known. To determine the source emissivity precisely, is, however, a relatively difficult task, as the beam parameters, such as the impulse current and time, the beam repetition rate, the spread, the scanning width and the scanning frequency have to be considered.

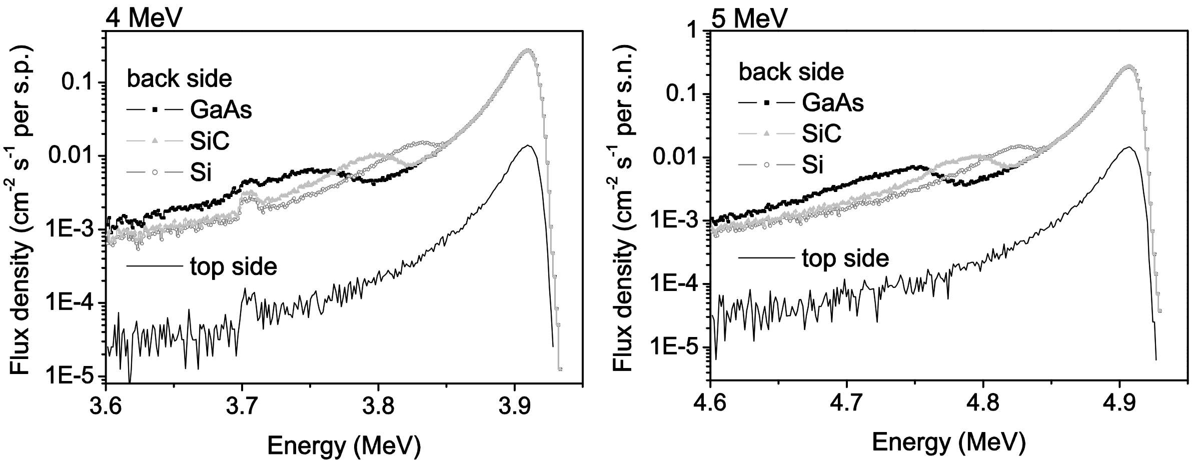

Fig.1: *Energy spectra on the detector top and back side surface after passing GaAs, SiC and Si detector volume. Energy of the incident electron beam was 4 (left) and 5 MeV (right).*

Tab. 1. *Results from MCNPX calculations for GaAs, SiC and Si detectors.*

Detector material	Energy of electrons [MeV]	F2 tally (flux density) $[cm^{-2}.s^{-1}$ per s.p.]	F6 tally (deposited energy) $[MeV.g^{-1}.s^{-1}$ per s.p.]	Dose rate $[Gy.s^{-1}$ per s.p.]
GaAs	4	0.307	0.207	$3.32\ .10^{-5}$
	5	0.317	0.216	$3.46\ .10^{-5}$
SiC	4	0.306	0.269	$4.31\ .10^{-5}$
	5	0.317	0.276	$4.42\ .10^{-5}$
Si	4	0.306	0.282	$4.52.\ 10^{-5}$
	5	0.317	0.287	$4.60\ .10^{-5}$

Finally, the dose depth distributions in GaAs, SiC and Si detectors irradiated by 4 and 5 MeV electron beams were simulated using type 1 mesh tally with PEDEP option. This tally scores the energy deposition by electrons within a mesh cell and the units are $MeV.cm^{-3}$ per s.p.. The mesh divided the 1 cm thick detector material into 20 layers, each of them 0.5 mm thick (the volume of the mesh cell was 8 mm^3). The distributions of deposited energies are shown in Fig. 2a. Typically, the dose depth curve exhibits a high surface dose followed by a build up region. After reaching the maximum, the dose drops off rapidly and levels off at a small low-level dose component referred to as the bremsstrahlung tail. The slope of the falloff region is larger for the heavier material, like GaAs and gentler for materials with smaller atomic weight, as Si and SiC. Generally, the absorbed dose remains unchanged and close to zero at the material thickness corresponding to the electron range. As obvious from the GaAs distribution, the deposited energy starts to increase toward the end of the investigated thickness. This behavior is caused by the electrons backscattered from the iron board, which contribute to the total deposited energy and consequently increase it. This explanation confirmed the simulation without the iron board (with air outside), where the absorbed energy leveled off, as expected (upper right hand corner in Fig. 2a). In Fig. 2b, a distribution of absorbed dose is plotted for GaAs irradiated by 4 MeV electrons. The square empty points in the graph represent the experimentally obtained values of absorbed dose. As obvious, a very good agreement between simulation and measurement was obtained.

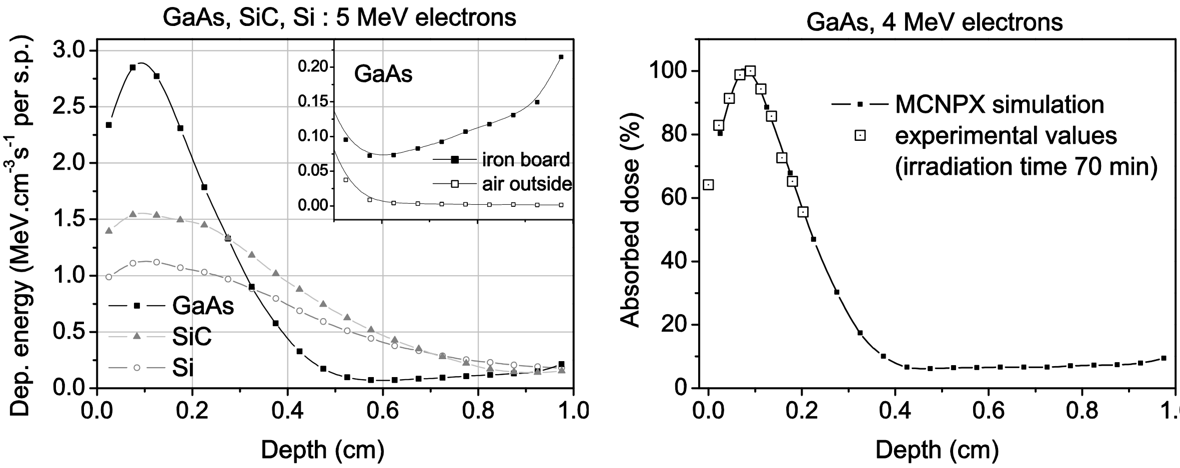

Fig.2: *Dose depth distribution in GaAs, SiC and Si detectors irradiated by a 5 MeV electron beam (a); comparison between the MCNPX simulation and the experiment for GaAs irradiated by a 4 MeV electron beam.*

5. Conclusion

This study aimed to treat some practical problems of (not only) semiconductor material irradiation by high energy electron beam using MCNPX simulation code. The relation between the absorbed dose and the fluency was found and the energy distribution of electron flux density was simulated on the top and back side of 270 μm thick GaAs, SiC and Si detectors. Furthermore, the dose depth profiles were calculated for GaAs, SiC and Si materials irradiated by 4 and 5 MeV electron beams. For the GaAs detector, a very good agreement with the experiment was shown. To match the absolute values of the absorbed dose with experimentally obtained values, the electron source emissivity has to be determined in relation to the electron beam setting parameters.

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