Simulation of MeV electron energy deposition in CdS quantum dots absorbed in silicate glass for radiation dosimetry

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Abstract. We are currently developing 2D dosimeters with optical readout based on CdS or CdS/CdSe core-shell quantum-dots using commercially available materials. In order to understand the limitations on the measurement of a 2D radiation profile the 3D deposited energy profile of MeV energy electrons in CdS quantum-dot-doped silica glass have been studied by Monte Carlo simulation using the CASINO and PENELOPE codes. Profiles for silica glass and CdS quantum-dot-doped silica glass were then compared.

1. Introduction

Recent studies have investigated the change in the optical response of quantum-dots contained in glass matrices as a function of the absorbed ionizing radiation dose. A variety of different techniques have been exploited, for example change in optical absorption [1], change in thermoluminescence [2] and, for quantum-dots in a liquid environment, the change in the optical-stimulated fluorescent yield [3].

In order to investigate electron irradiation of quantum-dot-doped silica glass, Monte Carlo simulations using the CASINO [4] and PENELOPE [5] software packages were carried out. With these simulations, the electron interactions in material are grouped and referred to using a multiple scattering theory [6]. In CASINO, the electrons trajectory is moving from the entry point through the material until their energy is absorbed or they are backscattered out of the material. CASINO is however limited to planar layer structures and does not simulate bremsstrahlung emission of photons explicitly. Mathematical models are applied to calculate the probability of the scattered electrons, the scattering angle, distance between scattering events and the energy rate loss. The more sophisticated Monte Carlo code PENELOPE enables the simulation of electrons, positrons, and photons in any material, in complex geometries, over the energy range of a few hundred eV to 1 GeV. The cross-sections acquired from both numerical databases and analytical models were used in scattering models for the different types of interaction mechanisms [7].

The motivation for this work was the development of new 2D imaging radiation dosimeters for electrons and photons up to a biologically important absorbed dose of a dose level commonly used in radiation therapy to high dose rate for industrial usage. There is considerable interest in dosimetric techniques which have either 2D/3D spatial information or the ability to be rapidly and remotely interrogated during an irradiation or both. Optical absorbance and fluorescence are both techniques which can provide this capability. In this work, we report on simulations with bulk and surface

absorbed quantum-dots in a silica matrix. A silica matrix was chosen as this material is highly radiation-tolerant to both electron and gamma irradiation and thus any changes in its bulk optical properties, critically absorption in our application, will be negligible at the doses we are using. Our initial aim is to investigate dosimeters, using near-UV excited fluorescence of the quantum dots, that are optically imaged onto a sensitive video camera to provide a two-dimensional dose map. The use of CdS-silica-CdS sandwich structures potentially allows some level of discrimination between electron and gamma irradiation as the dose-depth characteristics can be very different, different sized quantum dots could be used on the two surfaces to provide colour discrimination when the dosimeter is read out.

2. Monte Carlo Simulation

The two Monte Carlo simulation codes used in this work were CASINO and PENELOPE. Comparisons between silica glass only profiles with quantum-dot-doped silica glass were then made to investigate the depth dose distribution and the energy of backscattering electrons.

In both simulations, a 0.1cm slab of silica (SiO_2) glass was exposed to a beam of 1 MeV accelerating electrons. The source point is located at the sample surface and irradiates towards the sample. For the quantum-dot-doped silica glass simulation, the same geometries were considered with 1000 nm of CdS quantum-dots deposited on each face and a third geometry with the same ratio of CdS to SiO_2 but with the CdS uniformly distributed throughout the bulk silica matrix.

3. Results and Discussion

3.1. Depth-dose distribution

Figure 1 shows the dose distribution by PENELOPE over the sample's depth following irradiation by 1 MeV electrons. The dose grows a bit higher in CdS-Silica-CdS at the beginning and increases to a peak dose at 0.057 cm depth. In Silica, the dose is very slightly smaller than that in CdS-Silica-CdS with a peak also occurring at 0.057 cm depth. The scattering of primary electrons that lose energy along the path is responsible for the build-up zone.
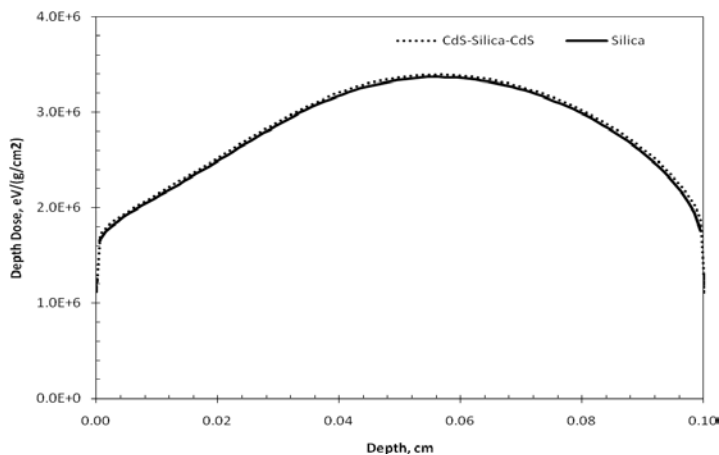

Figure 1. The depth-dose distribution in quantum-dots-doped silica glass (CdS-Silica-CdS) and silica glass only (Silica) from PENELOPE. The slabs were irradiated by 1 MeV accelerating voltage.

Figure 2 shows the distribution of penetration depth of backscattered electrons for quantum-dots-doped silica glass and silica glass only at 1 MeV by CASINO. 200000 electrons were used in each simulation to simulate the model. The backscattered electrons (BE) in CdS-Silica-CdS can travel through the sample further than in Silica. At a depth of 0.055 cm in Silica, the number of BE is starting to decrease and they have the potential to leave the sample surface. However, because of the fluctuations in the data, further analysis is required to interpret these data.
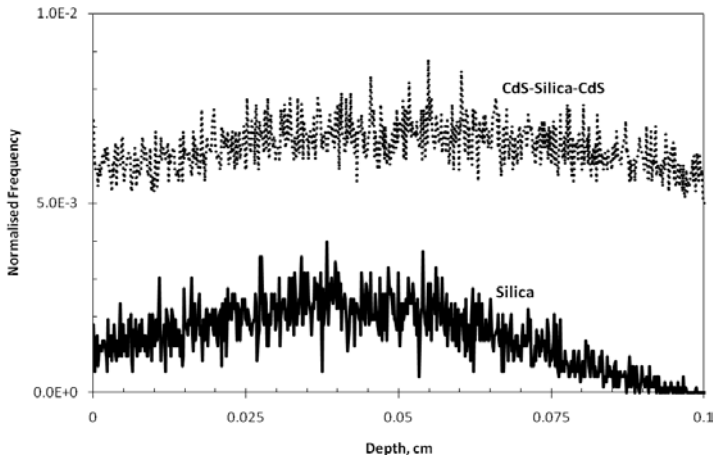
Figure 2. The maximum penetration depth of backscattered electrons in quantum-dots-doped silica glass (CdS-Silica-CdS) and silica glass only (Silica) by CASINO. The slabs were irradiated by 1 MeV accelerating voltage. The fluctuations reflect limited statistics. The CdS-Silica-CdS curve is multiplied by a factor of 5 for clarity.

Figure 3 shows the depth dose of porous Vycor glass with CdS quantum dots absorbed (Vycor-CdS) to compare to CdS-Silica-CdS. The thickness of the porous Vycor has been increased, compared to pure silica, because of its lower density.
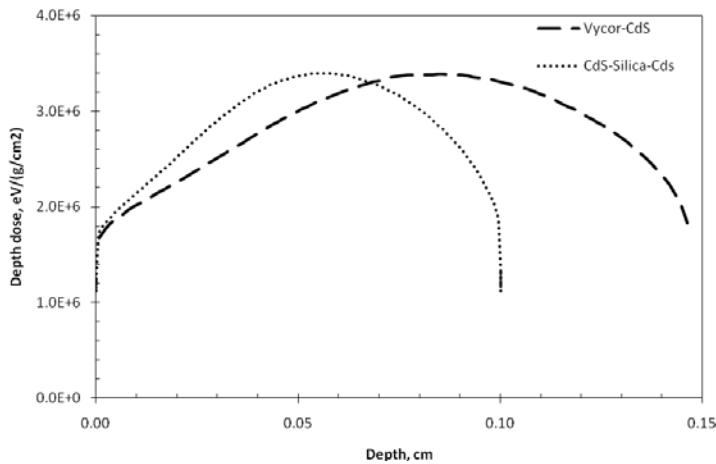

Figure 3. The depth-dose distribution in CdS quantum dots in Vycor glass matrix (Vycor-CdS) and quantum-dots-doped silica glass (CdS-Silica-CdS) from PENELOPE. The slabs were irradiated by electrons with 1 MeV accelerating voltage.
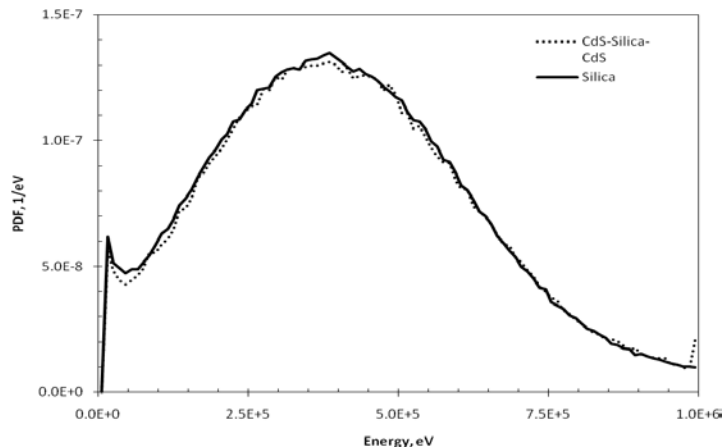
3.2. Backscattering electrons

Figure 4. The energy distribution of backscattered electrons in quantum-dots-doped silica glass (CdS-Silica) and silica glass only (Silica) from PENELOPE. The slabs were irradiated by electrons with 1MeV accelerating voltage.

Figure 4 and 5 show the energy of backscattered electrons when leaving the surface sample. In CASINO, there is no difference between two samples. Meanwhile, PENELOPE shows a more complex profile since it correctly takes into account bremsstrahlung photons as well as electrons and a small enhanced full energy backscatter peak is predicted for the CdS-Silica-CdS sample.
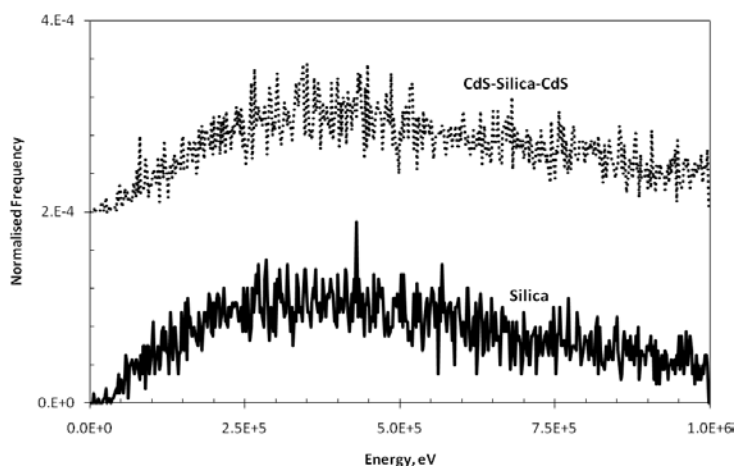

Figure 5. The energy of backscattered electrons in quantum-dots-doped silica glass (CdS-Silica-CdS) and silica glass only (Silica) from CASINO. The slabs were irradiated by electrons with 1 MeV accelerating voltage. The fluctuations reflect limited statistics. The CdS-Silica-CdS curve is multiplied by a factor of 2 for clarity.

Data from the CASINO simulations shown in Figures 2 and 5 are expressed in terms of 'normalised frequency' on the y-axis, the default output of CASINO, which provides measure of the frequency of occurrence of a particular process. In contrast, PENELOPE is able to provide output in terms of the specific energy deposited as a function of distance into a material, as in Figures 1 and 3, or as a probability distribution function, as in Figure 4.

4. Conclusion

Our preliminary results show that in terms of parameters such as backscattered electron spectra for 1MeV incident electrons CASINO and PENELOPE give similar, but not identical results. CASINO is not directly able to provide either a 1D or 2D profile of dose versus depth in contrast to PENELOPE. PENELOPE simulates processes involving photon emission and subsequent scattering and absorption which are absent from CASINO. This also enables PENELOPE to be used in applications where the incident radiation field consists of high energy gamma rays, such as those from ^{60}Co sources.

Our simulated results of layered CdS-Silica-CdS dosimeters have been compared with a possible dosimeter using quantum dots absorbed into a porous silica glass matrix, such as Vycor 7930 [8]. As expected, the differences in response are subtle but for some applications, lower energy incident electrons for example, or mixed radiation fields, they may be significant. The use of the PENELOPE Monte Carlo will enable us to model these effects more fully in our subsequent experimental work.

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