Modelling Optimal characteristics of a-Si:H Semiconductor Detectors For X-Ray Detection.

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Abstract-- The promising perspectives and important advantages of the amorphous silicon $p$-$i$-$n$ semiconductor detector for the direct detection of X-rays at room temperature, make them suitable for medical applications. In this work, photons in the mammographic energy range obtained from a Molybdenum target X-ray tube, were transported in an a-Si:H diode using MCNP-4C system code based on Monte Carlo method. The geometric features of $p$-$i$-$n$ type a-Si:H diodes grown with PECVD high deposition rate technique, whose spectrometric characterization was reported in a previous work, where included in our calculations. The energy deposition profile on a structured a-Si:H detector is evaluated and the calculations are carried out for devices whose intrinsic layer thickness was varied from 5 $\mu$m to 50 $\mu$m. The influence of the composition and thickness of four different contact electrodes on the energy deposition process inside the intrinsic layer is described in detail. Some physical parameters of these devices are estimated and discussed in order to increase the electron-hole quote production per incident photon on the intrinsic layer and get the best X-ray detection conditions.

Introduction

The extensive use of radiation detectors based on hydrogenated crystalline and amorphous $p$-$i$-$n$ silicon semiconductor devices, is more and more common in research based on nuclear techniques, being medical physics one of the fields where these devices have found enormous possibilities of use [1][2][3][4]. The growing interest of the international community and the promising perspectives of use of these devices, have lead to studies aimed to characterize the radiation detection properties and radiation damage resistance of hydrogenated silicon detectors. The hydrogenated amorphous silicon (a-Si:H) detectors have some important advantages over the similar crystalline ones and have become an active research field in recent years due to the possibility of extremely low fabrication cost, offering the possibility of growing much larger areas. Their compatibility to be integrated with read-out circuits is also important. The high radiation damage resistance capabilities of this kind of material are enhanced, making it possible to tolerate high doses without affectations.

The energy deposition profile inside an a-Si:H detector is evaluated by using the MCNP-4C code in this paper. The influence of the composition and thickness of the contact electrodes on the energy deposition process inside the intrinsic layer of the device is determined through the transport of photons in the energy range of an X-ray tube with Mo target. The geometric features of real Cr-a-Si:H $p$-$i$-$n$ detectors which were grown with PECVD high deposition rate technique, where included in our calculations. The spectrometric characterization of this devices was reported in a previous work [5][6].

Simulation by Monte Carlo

The MCNP code developed in Los Alamos[7] carries out the radiation transport calculations, with energy and time dependence in a three-dimensional geometry by using the Monte Carlo method. This method is based on the random sampling modelling of each transport event developed according a probability distribution function and consequently, the evolution of the particular phenomena being performed by means of convenient statistical techniques. The capabilities of this code involve the correct simulation of the physical problem and the choice of different geometrical configurations, as well.

On this basis, the MCNP-4C code calculations were applied in order to determine the X-ray deposited energy distribution, through a $p$-$i$-$n$ amorphous silicon diode structure, according to the simulated layer distribution shown in Fig.1. The square area is $65 \times 10^4$ cm$^2$, while the layer thicknesses are shown in the figure. Taking into account that the collection efficiency of the detector is affected by the thickness of the intrinsic layer, the calculation was made for diodes whose intrinsic layer thicknesses were varied from 5 $\mu$m to 50 $\mu$m. Both $p$- and $n$-layer were considered with the same width in all cases. In order to determine how the deposited energy is distributed...
inside the \(i\)-layer, calculations were performed by introducing \(i\)-sub layers of 0.2 \(\mu\)m. The doping of the \(p\)- and \(n\)-layers is achieved by adding the required amount of Boron (for \(p\)-type) and Phosphorous (for \(n\)-type) to get a concentration of 10\(^{18}\) atoms / cm\(^3\) or 0.00002 atoms per silicon atom in the sample, in both cases.

For our simulation we used the typical X-ray spectrum produced by a Senographe 700T X-ray clinical mammography system operated at about 28 kVp and based on a Mo target X-ray tube with a 0.03 mm Mo filter. The resultant photon energy spectrum shows characteristic fluorescence K-lines at 17.5 keV and 19.6 keV superimposed upon a bremsstrahlung background exhibiting a sharp reduction in intensities above 20 keV due to the absorption edge of the Mo filter. The focal point of the beam was considered at 60 cm over the top metal electrode, allowing the photons to impinge normally to it, resembling the conditions commonly employed in standard mammography diagnosis.

Photon and electron deposited energy calculation, as well as the integrated currents over different surfaces were computed with the appropriate tallies. In these Monte Carlo simulations, 10\(^7\) histories were run, providing an estimated relative error less than 5%, producing reliable confidence intervals. Furthermore, each calculation output was statistically examined through its fluctuation chart, where statistical parameters like Figure of Merit (FOM) were evaluated in order to improve statistically well behaved outputs.

No variance-reduction techniques were introduced, only conservative methods like the increasing of the number of histories, where applied in calculations. All diode geometry inside regions were declared equally important, regarding to photon and electron transport. Alternatively, the importance of the diode geometry outside space was set equal to zero.

Fig. 1. Schematic representation of the a-Si:H diode.

Our simulation, in order to analyse the behaviour of the deposited energy in the intrinsic layer of the Fig. 1 is performed by selecting a fixed thickness of 20 \(\mu\)m for the intrinsic layer and considering Chromium electrodes, the photon and electron transport was carried out throughout all the a-Si:H diode structure. The behaviour of the energy deposited in the different components of the device is shown in Fig. 2. As it can be seen in this figure, the X-ray deposited energy in the a-Si:H detector shows two main issues: a) the highest values of the deposited energy are reached at the extreme metal layers, b) a flat linear minimum exists in the central \(i\)-layer. This behaviour relies on the characteristic features of the photoelectric effect, the ratio of the maximum deposited energy value per depth length on the Cr-electrode to its minimum value on the \(i\)-layer is very close to the ratio of the relative total photoelectric cross section values from Cr and Si atoms

\[
\frac{\rho_{Cr}}{\rho_{Si}} \left( \frac{Z_{Cr}}{Z_{Si}} \right)^{5} \]

where; \(\rho\) and \(Z\) are the density and atomic number of the respective element.

Fig. 2. Simulation of the deposited energy per incident photon in the diode as function of depth in all the device components.

Since the contribution of the photoelectric ionisation absorption process to the deposited energy must decay monotonically with the penetration depth, most of the features of the deposited energy in depth distribution shown in Fig. 3 are due to contributions caused by the photo excited secondary electrons produced at any layer, which can penetrate and interact with the other neighbour layers. In particular, the non-linear increase of the deposited energy from the inner layers (\(p\)-, \(n\)-layers and the \(i\)-sub layers close to them) to the contact electrodes depends on the number of ejected electrons, \(N_e\), from the metal layer, which can penetrate up to the borders of the \(i\)-layer, according to the value of the free scattering length \(\lambda_e\) of the secondary electrons.

The \(N_e\) value at a given X-ray energy will depend on the atomic composition of the metallic layer as well as the thickness, and has a substantial contribution to the deposited energy in the intrinsic layer.
The influence of the contact electrode thickness on $N_e$ is presented in Fig. 4. Here, four different elements were used for the contact electrode (Al, Cr, Mo, Pd) and the thickness of the top electrode was varied, starting from 0.01 µm.

This simulation was made for all possible electron trajectories crossing the boundary surface between the metal layer and the doped (n or p) silicon layers, where $N_e$ was normalized per X-ray incoming photon.

As it was expected for photoelectric effect, $N_e$ becomes higher for heavier metals (Pd) than for light metals (Al). At a given composition of the top electrode, $N_e$ initially increases with the metal layer thickness, reaching a maximum at a given optimal thickness ($t_0$), whose values are shown in Table I. For $t > t_0$, $N_e$ decays due to the increment of the self-absorption, where the initially photo excited electrons at the contact electrode will undergo multiple scattering events losing their energies. Hence, only a part of the ejected electrons will leave the contact electrode and will arrive at the $i$-layer until a penetration depth according to the mean free scattering lengths in the silicon layers.

For the bottom metal electrode, there is also an important contribution of those photoelectrons that are scattered at large angles to the silicon layers. See Fig. 5. The increase of this photoelectrons is more pronounced up to an electrode thickness of ~0.7 µm, after that, an asymptotic behaviour is reached.

Thus, the total deposited energy $E_{dep}(i)$ in the $i$-layer will comprises the following two main contributions: a) the energy $E^p_{dep}$ being deposited by the X-ray flux $N_p$, transmitted through the top contact electrode, b) the deposited energy $E^e_{dep}$, related to the penetration into the $i$-layer of the photoelectrons being ejected from the metal contacts, where both, the top and the bottom contacts are involved. Therefore,

$$E_{dep}(i) = E^p_{dep}(N_p) + E^e_{dep}(N_e)$$

### Table I. Top electrode thickness for which the maximum electron yield is attained.

<table>
<thead>
<tr>
<th>Top electrode material</th>
<th>Z</th>
<th>Thickness for maximum electron yield $t_0$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminium</td>
<td>13</td>
<td>&gt; 1.3</td>
</tr>
<tr>
<td>Chromium</td>
<td>24</td>
<td>1</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>42</td>
<td>1.2</td>
</tr>
<tr>
<td>Palladium</td>
<td>46</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Fig. 3. Simulation of the deposited energy per incident photon in the silicon layer of the diode. In this case a diode with a 20 µm thick intrinsic layer was considered. The $i$-layer was divided in 0.2 µm thick sub layers.

Fig. 4. Simulation of electrons outgoing the top metal electrode into the silicon layer. Influence of electrode thickness and its atomic number.

Fig. 5. Simulation of electrons outgoing the bottom metal electrode into the silicon layer. Influence of electrode thickness and its atomic number.
where \( N_p \) decays exponentially with the metal layer thickness, being 120 – 130 times higher than \( N_p \) at the metal thickness \( t_0 \) for the heavier metals. The photon to electron rate for different thickness values of the top metal electrode is shown in Fig. 6.

![Fig. 6. Photon / electron ratio crossing the surface that divides the top metal and p silicon layer.](image)

The relative contribution of \( E_{dep}^P \) in the Eq. 1 increases and becomes dominant when the \( i \)-layer thickness is greater than the penetration length \( \lambda_e \) of the ejected electrons from the metal into the intrinsic layer.

The above represented electron number \( N_e \) from the top electrode reaches a maximum value at \( t_0 \), whereas \( E_{dep}(i) \) shows also a maximum, as it is shown in Fig. 7, at some metal layer thickness \( t_0' < t_0 \) where the transport was made for an \( i \)-layer of 20 \( \mu m \) thick. For this thickness (\( \gg \lambda_e \)) the \( t_0' \) values are shown in Table II by simulating different metal compositions. Both \( t_0' \) and \( t_0 \) values were also calculated for the same 20 \( \mu m \) thick diode (see also Table I).

![Fig. 7. Influence of top electrode thickness on the total deposited energy in the intrinsic layer. In this case a diode with a 20 \( \mu m \) thick intrinsic layer was chosen and four different metals were considered as electrode contacts.](image)

<table>
<thead>
<tr>
<th>Top electrode material</th>
<th>Z</th>
<th>Optimal thickness ( t_0' ) (( \mu m ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminium</td>
<td>13</td>
<td>1.0</td>
</tr>
<tr>
<td>Chromium</td>
<td>24</td>
<td>0.7</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>42</td>
<td>0.7</td>
</tr>
<tr>
<td>Palladium</td>
<td>46</td>
<td>0.5</td>
</tr>
</tbody>
</table>

There is a similar contribution of the photoelectrons from the bottom metal electrode to the deposited energy in the intrinsic layer. However, the very dominant \( E_{dep}^P \) contribution to \( E_{dep}(i) \), near the proximity of the bottom electrode makes the influence of the metal thickness variation to be negligible, as is shown in Fig. 8, where a change of electrode thickness from 0.5 \( \mu m \) to 1 \( \mu m \) causes a variation of less than 1 % on the deposited energy inside the intrinsic layer, and from this point the deposited energy is almost constant in spite of the bottom electrode thickness.

![Fig. 8. Influence of bottom electrode thickness on the total deposited energy in the intrinsic layer. In this case a diode with a 20 \( \mu m \) thick intrinsic layer was chosen and four different metals were considered as electrode contacts.](image)

In Fig. 9, the dependence of the deposited energy in the intrinsic layer with respect to its thickness is illustrated. In this case, the simulation was carried out with the same 0.5 \( \mu m \) thick metallic electrodes and the thickness of the intrinsic layer was varied from 5 \( \mu m \) to 50 \( \mu m \). The total deposited energy in the intrinsic layer shows a linear relationship with the thickness, as expected.

In fact, the improvement of the detector efficiency is expected as the thickness of the intrinsic layer is increased, but this approximation is constrained because of the huge values of reversed voltages (various kV) applied to the \( p-i-n \) diodes to achieve the complete electric charge depletion in that layer,
which may provoke the break-down of the device. Also, the deposited energy in the doped layers was calculated (data not shown), but it was not sensitive to the increasing of the intrinsic layer thickness.

To obtain the best X-ray detection efficiency by increasing the number of electron-hole pairs per incident photon on the i-layer, the top electrode contact thickness must vary between $t_0’$ ($\approx 0.7$ µm) and $t_0$ (1.0 µm) and the bottom electrode thickness must be preserved in the reasonable range from 1 µm to 2 µm.

### III. CONCLUSIONS

Monte Carlo X-ray transport calculations with the MCNP code were applied on a structured a-Si:H detector and it has been proved to be suitable for describing in details its energy deposition profile.

As a result of present calculations, the influence of contact electrode composition and thickness on the energy deposition process has been analysed. The correlation between the relative weights of the i-layer deposited energy by the transmitted X-ray flux $N_{ph}$ into that from the metal layer ejected electrons into the i-layer has been studied.

In particular, it has been concluded that palladium, chromium, and molybdenum contacts show similar characteristics regarding to the deposited energy in the intrinsic layer and can be suitably employed as electrodes to be used in a-Si:H detectors to get optimum energy deposition profile.

### IV. REFERENCES


