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New Numerical Method to Calculate the True Optical Absorption of Hydrogenated Nanocrystalline Silicon Thin Films

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ABSTRACT

The enhanced optical absorption measured by Constant Photocurrent Method (CPM) of hydrogenated nanocrystalline silicon thin films is due mainly to bulk and/or surface light scattering effects. A new numerical method is presented to calculate both true optical absorption and scattering coefficient from CPM absorption spectra of nanotextured nanocrystalline silicon films. Bulk and surface light scattering contributions can be unified through the correlation obtained between the scattering coefficient and surface roughness obtained using our method.

Keywords: Solution Hydrogenated Nanocrystalline Silicon; Constant Photocurrent Method; Optical Absorption; Bulk Light Scattering; Surface Roughness; Film Thickness

1. Introduction

Materials with nanometer crystallites constitute an important class with some of their properties distinctly different from either amorphous or large grain materials or single crystals. Especially, hydrogenated nanocrystalline and polymorphous silicon thin films. Hydrogenated nanocrystalline silicon (nano-Si:H) is an heterogeneous material. It consists of an ordered nanocrystallites of spherical form with size varies from 2 to 100 nm embedded in amorphous matrix [1]. These semiconducting nanomaterials are very promising to the photovoltaic applications [2]. The important key for the success of nano-Si:H films as a PV absorbent materials is their enhanced absorption compared to the monocrystalline silicon (c Si), mainly in infrared region [3]. The main reason of this optical behavior is due to their particular structure which gives place to the bulk and/or surface light scattering phenomena [3-5]. The Constant Photocurrent Method measurements of these heterogeneous mediums give us an "apparent" optical absorption coefficient $\alpha_{app}(E)$ at energy *E*. $\alpha_{app}(E)$ is affected by light scattering effects different from α_{true} measured for homogeneous mediums, *i.e.*, amorphous or monocrystalline silicon [3]. In this paper, we suggest a new numerical method to calculate the true optical absorption. A numerical resolution of Equation (1) is given at energy $E = 1.1$ eV. The contribution of bulk light scattering, from the spectral dependence of apparent optical absorption coefficient $\alpha_{app}(E)$ in thin films of nano-Si:H is measured by Constant Photocurrent Method (CPM). The details of CPM method and its experimental configuration are described elsewhere [6]. This method is developed in order to understand the subgap part of the true optical absorption spectra related to the defect states within the energy gap. It's introduced with the help of a recent theory [3] which describes the different contributions of light scattering in terms of photocurrent (I_{Ph}) deduced from CPM measurements. This procedure has a crucial importance to determine α_{true} in the case of weak bulk light scattering, without need to compare a several CPM measurements (for different interelectrodes spacing) [3]. We will present the details of our procedure and discuss its validity by comparing a calculated $\alpha_{true}(E)$ spectrum with the experimental one obtained by CPM for the same sample of nano-Si:H. Finally, we will apply this method on a series of nano-Si:H which have a different surface roughness in order to determine the correlation between this material parameter and the scattering coefficient α_{sc}.

2. Numerical Method

In the following, let us consider a nano-Si:H thin film with a typical thickness d_f configured according to the CPM setup. If the standard CPM evaluation method will be applied to the measured spectrum, we will obtain an "apparent" optical absorption coefficient α_{app} for which the following equation is valid [3]:

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$$\left[1-\exp\left(-\alpha_{app}\cdot d_f\right)\right]-\frac{1}{\alpha_f}\left[1-\exp\left(-\alpha_f\cdot d_f\right)\right]$$
$$\times\left\{\alpha_{true}+\alpha_{sc}\cos\theta\left[1-\exp\left(-\frac{\alpha_{true}}{\alpha_{sc}}\right)\right]\right. \tag{1}$$
$$\left.\times\frac{\left[\cos\theta\,\exp\left(-\frac{\alpha_{true}}{\alpha_{sc}}\right)\right]^{N_{bulk}}-1}{\left[\cos\theta\,\exp\left(-\frac{\alpha_{true}}{\alpha_{sc}}\right)\right]-1}\right\}=0$$

where α_f is the total optical absorption in the film given by:

$$\alpha_f=\alpha_{sc}+\alpha_{true} \tag{2}$$

N_{bulk} is the number of the scattering events between the electrodes (to calculate this parameter see reference [3]) and θ is the critical angle for total reflections. θ defines the escape cone and can be calculated from the total internal reflection condition $\sin\theta=n/n_f$, where n is the refractive index of the outer medium. The function "cosθ" presents the propability that the incident photon is scattered outside the escape cone. The parameters, α_f and θ are known experimentally. We have considered the experimental values measured by the authors of the reference [3], in order to compare our method with their experimental one. We have taken cosθ = 0.5 calculated for 2 µm thick nano-Si:H with an spectrum measured by CPM method for 8 × 2 mm interelectrode spacing (**Figure 3**). The Equation (1) (with the variable α_{sc}) cannot be solved analytically and an adequate numerical method will be used.

First, we give some estimated values for the true optical absorption coefficient α_{true}, and we inject them in Equation (1) in order to get a solution. We must take into account that $\alpha_{app}(E)>\alpha_{true}(E)$.We note that for each $\alpha_{app}(E)$ value, it corresponds a $\alpha_{true}(E)$ value at the considered energy. After that, we choose the limited α_{true} values (minimum and maximum values) in order to get an $\left[\alpha_{sc,\min},\alpha_{sc,\max}\right]$ interval. For each interval of α_{true} values, it corresponds an interval of α_{sc} values $\left[\alpha_{sc,\min},\alpha_{sc,\max}\right]$. Second, in order to calculate values with a good precision at the considered energy, we select the α_{true} values in which the interval $\left[\alpha_{sc,\min},\alpha_{sc,\max}\right]$ will be much reduced. It means that α_{true} values which favour the following condition:

$$\frac{\alpha_{true,\max}-\alpha_{true,\min}}{\alpha_{true,\max}+\alpha_{true,\min}}\le 1\% \tag{3}$$

Finally, we calculate the mean value $\alpha_{true,mean}$ of the selected interval and we replace it in Equation (1) in order to determine the corresponding solution α_{sc}. **Figure 1** shows the numerical resolution of Equation (1) according to this process. After that, we suppose that the spectral dependence of the calculated scattering coefficient has the following form in the energy range which favours the previous inequality:

$$\alpha_{sc}(E)=\beta E^{\gamma} \tag{4}$$

where β and γ are a constants.

Using the values of $\alpha_{sc}(E)$ at energy E estimated in the first step and by a simple convolution, we can determine the constants β and γ (**Figure 2**).

In **Figure 2**, one can observe that the convoluted spectrum of scattering coefficient corresponds to the Rayleigh type of scattering, *i.e.*, a dependence of E^4. Consequently, $\alpha_{sc}(E)$ can be calculated in all the considered energy

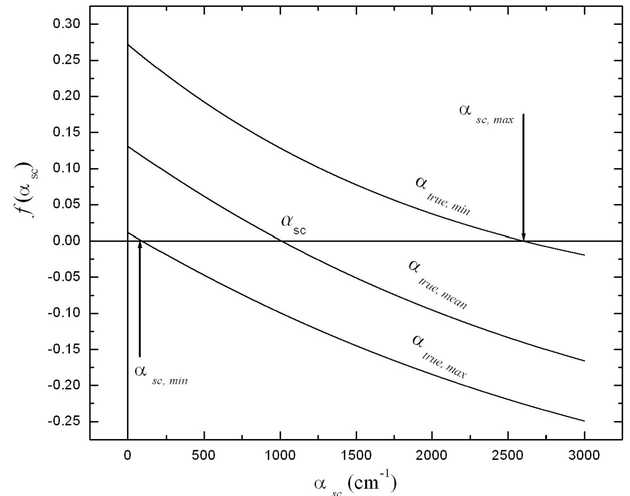

Figure 1. Numerical resolution of Equation (1) given at energy E = 1.1 eV.

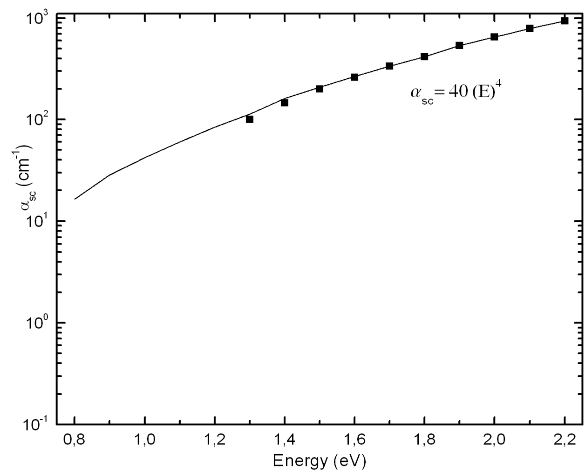

Figure 2. Convoluted $\alpha_{sc}(E)$ spectrum in all considereted energy range.

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range. Then, we inject $\alpha_{sc}(E)$ values in Equation (1) but this time with variable α_{true} in order to calculate the spectral dependence of $\alpha_{true}(E)$. However, in reference [3], the authors have their specific experimental procedure to extract $\alpha_{true}(E)$ and $\alpha_{sc}(E)$ spectra of nano-Si:H samples. Indeed, they estimate the scattering coefficient from a comparison of several CPM measurements (for different interelectrodes spacing) [3,7] and they supposed a Rayleigh light scattering. Using the first equation and by an iterative procedure, they obtained the true optical absorption spectrum $\alpha_{true}(E)$. **Figure 3** shows a perfect agreement of the calculated and measured true optical absorption coefficient spectra.

3. Experiment

Nanocrystalline silicon layers were deposited by RF magnetron sputtering of a silicon target, under different pressure (2, 3 and 4 Pa) with different substrate temperature (100˚C, 150˚C, 200˚C). This process enables to deposit the silicon thin films on all types of substrates. With respect to the deposition conditions, the layers result in a rough (textured). The measured typical root mean square surface roughness (σ_{rms}) of the nanotextured silicon samples varies between 4 and 12 nm. The CPM results of nano-Si:H series deposited at 2 Pa are shown in **Figure 4**.

We note that σ_{rms} of this series is about 6 nm for about 2.5 µm thick films. In order to exclude the influence of surface light scattering on the calculations, we have polished numerically the surfaces of the samples.

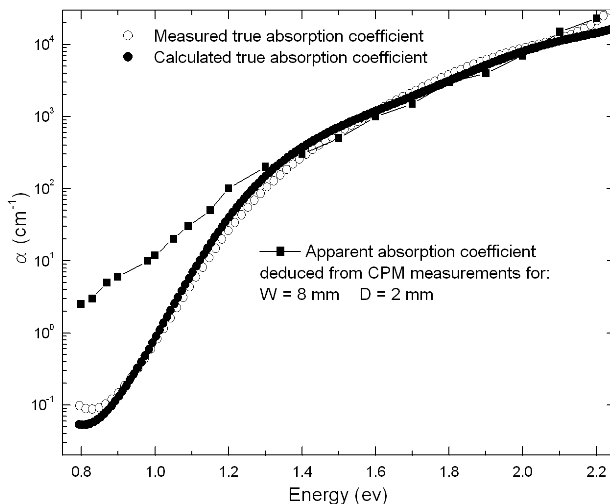

Figure 3. Comparison of true optical absorption spectra of thin nano-Si:H film deposited by Very High Frequency Glow Discharge (VHFGD) method. The results plotted by black bolls correspond to the values calculated by our numerical method and that plotted by empties bolls for α_{true} evaluated by the authors using their experimental procedure [3].

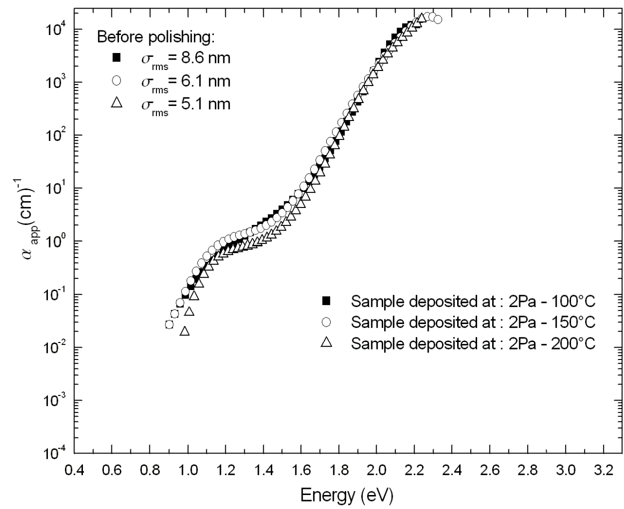

Figure 4. Fitted apparent optical absorption spectra of nano-Si: H series deposited by RF magnetron sputtering method under different substrate temperature. $\alpha_{app}(E)$ values are calculated after a numerical polishing of the film surface (σ_{rms} = 0 nm).

The polishing procedure has been done using the surface light scattering theory presented in reference [3]. Indeed, in the calculations, we have supposed that the textured Si has a smooth surface (σ_{rms} = 0 nm) and we have calculated $\alpha_{true}(E)$ values which are in reality the apparent optical absorption coefficient $\alpha_{app}(E)$ values influenced only by bulk light scattering effects (**Figure 4**).

The evaluated $\alpha_{app}(E)$ values will be after that, injected in our program in order to calculate $\alpha_{true}(E)$ and $\alpha_{sc}(E)$ spectra.

4. Results

We have applied our numerical method on the silicon series with their CPM data given in **Figure 4**. **Figure 5** shows the calculated spectral dependence of the true optical absorption $\alpha_{true}(E)$ and the scattering coefficient $\alpha_{sc}(E)$ of the sample deposited at 200˚C.

The calculated spectra of the samples of this series are presented together in **Figure 6**.

5. Discussions

Results presented in **Figure 5** and **Figure 6** demonstrate that the samples deposited at 2 Pa exhibit an important bulk light scattering contribution especially in low absorption range (0.9 - 1.6 eV spectral region) compared with the samples deposited at 3 and 4 Pa. These samples have a considerable surface roughness, which leads to a remarkably surface light scattering. Consequentially, the contribution of the scattered light at the rough surface will be dominant. Furthermore, the scattering coefficient

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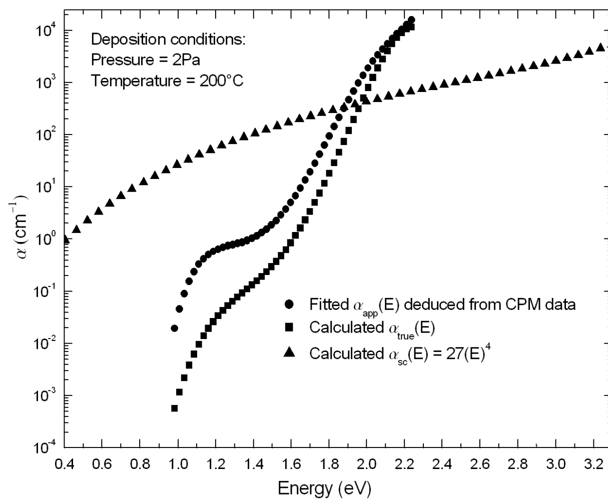

Figure 5. Scattering and true optical absorption spectra calculated from CPM data of nano-Silicon thin film deposited under pressure of 2 Pa and substrate temperature of 200˚C.

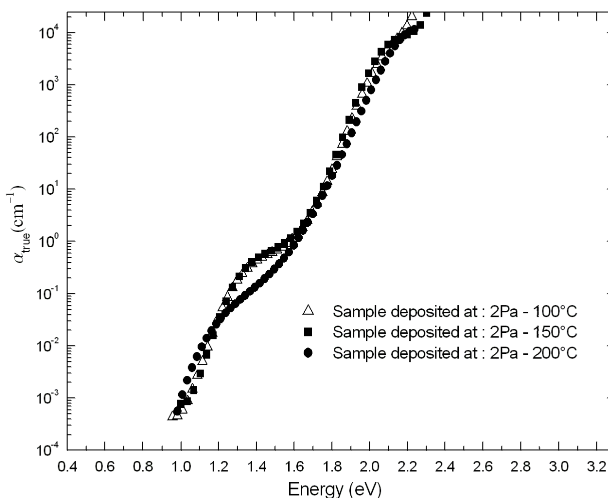

Figure 6. True optical absorption spectra calculated by the numerical method for a nano-Si:H samples deposited by RF magnetron sputtering method under different substrate temperature.

α_{sc} evaluated for each sample deposited at 2 Pa has the Rayleigh scattering form $\left(\alpha_{sc} \propto E^4\right)$. This result is very convenient with the nature of our sample. Indeed, we study here nanotextured thin films, *i.e.*, samples which have a random rough surface with rms roughness smaller than the wave length of the incident light. Furthermore, they possess the property to have small heterogeneities included in their volume similarly to the case of amorphous silicon. We must note that there are some nano-Si:H rough samples which demonstrate an important surface scattering and by a standard mechanical polishing, the surface scattering disappears and the true optical absorption is directly measured by CPM. But there are some other ones which exhibit a bulk scattering contribution, which cannot remove by polishing. We calculate their true and scattering coefficients spectra using the proposed numerical method. We can unify the bulk and surface scattering in terms of the scattering coefficient α_{sc} given by the following equation:

$$\alpha_{sc} = \frac{1}{d_f}\left(\frac{2\pi\left(n_f - n_a\right)\sigma}{\lambda}\right)^2$$

where n_f and n_a are respectively, the refraction indexes of nano-Si:H film and the ambient. λ is the incident wave length.

6. Conclusion

In this paper, we have developed a new numerical method in order to calculate the true optical absorption spectra and the contribution of light scattering in CPM measurements of hydrogenated nanocrystalline silicon thin films. With the help of surface and bulk light scattering theories presented by Poruba and al, we have concluded that the contribution of bulk light scattering in CPM spectra of nanocrystalline silicon samples deposited at low pressure which have a low surface roughness is due mainly to the included heterogeneities (nanocrystallites, voids,···) similarly to the case of amorphous silicon.

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