Monte Carlo simulation of surface light scattering in nanocrystalline silicon thin films and solar cells

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Résumé - L’absorption optique élevée mesurée par la Méthode de Photocourant Constant (CPM) des couches de silicium nanocristallin hydrogéné est due principalement au long chemin optique suivi par les photons diffusés sur la surface rugueuse des couches texturées. Nous avons essayé de simuler ce phénomène optique en étudiant l’influence de l’épaisseur de la couche de Si nanocristallin hydrogéné sur son absorption optique. Cette simulation est basée sur les méthodes de Monte Carlo. Nous avons conclu que l’absorption optique est inversement proportionnelle à l’épaisseur de la couche dans la gamme des faibles énergies. Ce résultat est très utile dans les applications photovoltaïques. La diffusion de la lumière sur une surface rugueuse est la clé caractéristique d’une cellule solaire efficace.

Abstract - The enhanced optical absorption in nanocrystalline silicon films analysed by Constant Photocurrent Method (CPM) mainly in infrared region is due a longer optical path as a result of an efficient diffuse light scattering at the textured film surface. We tried to simulate this phenomenon by introducing the influence of the film thickness on the optical absorption. This simulation is based on Monte Carlo methods. It pointed to the conclusion that the optical absorption is inversely proportional to the film thickness. This result is very promising in photovoltaic applications. Surface light scattering effect is a key characteristic of efficient thin-film-silicon solar cells.

Keywords: Optical absorption - Film thickness - Surface light scattering - Monte Carlo simulation - Solar cells.

1. INTRODUCTION

Hydrogenated nanocrystalline silicon (nano-Si:H) films are considered as heterogeneous mediums [1]. They consist of ordered nanocrystallites silicon which have a spherical form included in amorphous matrix [2]. These nanomaterials deposed by Plasma Enhanced Chemical Vapor Deposition PECVD at low temperature (<300°C) constitute an important class with some of their properties distinctly different from either amorphous or large grain materials or single crystals.

Moreover, they present a low metastability during their prolonged exposure to the light, compared with hydrogenated amorphous silicon (a-Si:H), which is very promising to the photovoltaic applications.

The important key for the success of the hydrogenated nanocrystalline silicon (nano-Si:H) layers as a PV absorbent materials is its enhanced absorption compared to the monocrystalline silicon, mainly in weak energies range. The main reason of this optical behavior is due to its particular structure, which gives place to the bulk and/or surface...
light scattering phenomena. Indeed, the photon trapped by the included nanocrystallites undergoes a several scattering events until its light intensity will attenuate, and consequently, it will be absorbed completely in its optical mean free path traveled during its scattering.

The CPM measurements of these heterogeneous mediums give access to an ‘apparent’ optical absorption coefficient affected by scattering effects different from that measured for the homogeneous mediums. The CPM well known from the field of amorphous silicon [3, 4]. It detects the light absorbed (either directly or after one or more scattering events) in between two metal electrodes used for the photocurrent measurements.

In this study, we will discuss the influence of different characteristic parameters of a heterogeneous material, (polymorphous or nanomaterial) especially the film thickness on its optical behavior by introducing a numerical simulation based on Monte Carlo methods. We will take into account the diffusive aspect of the characterized material.

2. SIMULATION METHOD

First, we consider a thin nano-Si:H film with a typical thickness $d_f$ deposited in-between two coplanar electrodes with width $W$ and distance $D$ [4]. We assume that nano-Si:H film is composed of a similar square lattices set equidistant of a distance ‘$L$’.

Each plan contains nanocrystallites of identical size, which constitute the diffuser sites in the sample (Fig. 1). Homogeneous matter of the film is represented by no-diffuser sites. Note that the distribution of the nanocrystallites on each plan is purely random but their number remains always fixed.

![Fig. 1: Square lattice of a nanocrystalline silicon layer configured according to the CPM setup](image)

Second, we suppose that the incident photon falls randomly on the site of the first plan. If this site is no-scatterer, the photon penetrates in the sample and passes in the second plan on the site located just below the first.

If the second site is also no-scatterer, the photon passes in the third plan and so on, until it crosses completely the film thickness. Consequently, the total film absorptance is equivalent to the true one given by the Beer’s law [5]:
where $\alpha_{\text{true}}$ is the true optical absorption coefficient in the film and $R$ is the reflectance.

If we use this simple approach (Beer’s law) for bulk and/or surface light scattering in the films, i.e., neglecting the changes in the spectral dependence of reflection $R(E)$ comparing with changes in $\alpha$ over several orders of magnitude, the attenuation of the specular beam will be given by:

$$A_{\text{true}} \approx 1 - \exp(-\alpha_{\text{true}} \times d_f)$$

However, if during its crossing the sample, the photon from the specular beam falls onto a scatterer site belongs to one of the sample plans, it will scatter randomly on the plan and in the space in all the directions, i.e., isotropic scattering, until its intensity will be attenuated (lower than $10^{-6}$ of its initial intensity) and it will be absorbed. If it is not absorbed, it will be scattered again and the same considerations are valid.

Therefore, the film absorptance for the scattered photon will be:

$$A_{\text{sc}} \approx 1 - \exp\left(-\alpha_{\text{true}} \times \text{Path}(i)\right)$$

where $\text{Path}(i)$ represents the mean free path traveled by the scattered photon $(i)$.

However, the total film absorptance of scattering nano-Si:H samples is defined as:

$$A_{\text{tot}} \approx \left(1 - \exp(-\alpha_{\text{app}} \times d_f)\right)$$

where $\alpha_{\text{app}}$ is the apparent optical absorption coefficient in the film measured by CPM.

On the other hand, CPM uses the photocurrent $(I_{\text{ph}})$ proportional to the amount of light absorbed in the film. Thus, taking into account the contribution of the scattered light to the CPM signal $I_{\text{ph}}$ will be composed of two components:

$$I_{\text{ph}} = I_{\text{true}} + I_{\text{sc}}$$

$I_{\text{true}}$ is proportional to $A_{\text{true}}$, it represents the photocurrent excited by the photons absorbed directly from the specular beam, i.e., without any scattering.

$$I_{\text{true}} \approx N_1 \times A_{\text{true}} \approx N_1 \left(1 - \exp(-\alpha_{\text{true}} \times d_f)\right)$$

$N_1$ is the number of no-scattered photons.

The component $I_{\text{sc}}$ represents the contribution of the photons absorbed after one or more scattering events. It is given by:

$$I_{\text{sc}} \approx \sum_{i=1}^{N_2}\left[1 - \exp(-\alpha_{\text{true}} \times \text{Path}(i))\right]$$

Here $N_2$ represents the number of scattered photons.

From the formulas 5, 6 and 7, we can write:
N\left[ 1 - \exp(-\alpha_{\text{app}} \cdot d_f) \right] \approx N_1 \left[ 1 - \exp(-\alpha_{\text{true}} \cdot d_f) \right] + \sum_{i=1}^{N_2} \left[ 1 - \exp(-\alpha_{\text{true}} \cdot \text{Path}(i)) \right] \tag{8}

Consequently, $\alpha_{\text{app}}$ values can be calculated easily from the formula 8:

$$\alpha_{\text{app}} \approx -\frac{1}{d_f} \ln \left[ 1 - \frac{N_1 \left[ \exp(-\alpha_{\text{true}} \cdot d_f) - 1 \right] + \sum_{i=1}^{N_2} \left[ \exp(-\alpha_{\text{true}} \cdot \text{Path}(i)) - 1 \right]}{N} \right] \tag{9}$$

Nevertheless, film transmittance is expressed as:

$$T_f \approx \frac{N_1}{N} \cdot \exp(-\alpha_{\text{true}} \cdot d_f) \tag{10}$$

3. RESULTS AND COMPARISON

The dependence of the calculated $\alpha_{\text{app}}(E)$ spectra on the film thickness is clearly shown in figure 2, mainly in the 0.8 - 1.1 eV spectral region.

![Figure 2: Calculated spectral dependence of $\alpha_{\text{app}}(E)$ of a nanocrystalline silicon layer as a function of the film thickness. The fitted spectral dependence of $\alpha_{\text{true}}(E)$ deduced from CPM measurements [6] is shown for comparison.](image)

The analysis of this figure shows that $\alpha_{\text{app}}$ values are inversely proportional to $d_f$. This result is in agreement with that found in experiments [6, 7] and in figure 3.
This one presents $\alpha_{\text{app}}(E)$ spectra deduced from CPM measurements and calibrated as well as with those obtained from Photoothermal Deflection Spectroscopy (PDS) and Transmittance and Reflectance (T/R) measurements for different class of nanocrystalline silicon samples which have different surface roughness (nanotextured samples) and film thickness deduced by Spectroscopic Ellipsometry Measurements obtained in our laboratory.

The samples were deposited by RF magnetron sputtering of a silicon target, under different pressure (2, 3 and 4 Pa) with substrate temperature 150 °C. This process enables to deposit the silicon thin films on all types of substrates.

The layers results in a nanotextured (rough). The measured typical root mean square surface roughness ($\sigma_{\text{rms}}$) varies between 6 and 16 nm. We note that the CPM spectra of samples deposited at 3 Pa and 4 Pa are completely different from that of sample deposited at 2 Pa.

Moreover, the $\alpha_{\text{app}}(E)$ spectrum measured for 2 Pa presents an aspect like that of standard amorphous silicon. However, the aspects of 3 Pa and 4 Pa spectra demonstrate the nanocrystalline character of our samples with a high optical absorption values in all the spectral range.

The nanocrystalline signature of the CPM spectra is due to the big nanocrystallites with size close to the film thickness (these results are confirmed as well with Raman spectroscopy and Ellipsometry measurements).

3. DISCUSSION

Results in figures 2 and 3 for nanotextured-Si:H samples demonstrate the influence of the film thickness on the calculated $\alpha_{\text{app}}(E)$ spectra. As a special study, we discuss here the surface light scattering effects by varying this parameter. The presence of big
nanocrystallites (aggregate composed of small nanocrystallites) with size comparable with the film thickness leads to an important roughness of the film surface. This dependence was confirmed in figure 3, where we can see that $\sigma_{\text{rms}}$ values increase with the decrease of $d_f$.

However, we shall note that the decrease of film thickness neglect the presence of small nanocrystallites in the bulk and consequently, to a negligible bulk light scattering. Therefore, surface light scattering will be the dominant phenomenon. Hence, the enhanced optical absorption is mainly due to the light scattering only at the rough surface. However, the photons scattered from the specular beam by the rough surface will be absorbed within the area between the electrodes. And thus, it will contribute to the CPM signal.

On the other hand, in figure 3, the $\alpha_{\text{app}}(E)$ spectra subsist also towards the weak energies with optical absorption attributed to broken bonds due to the amorphous fraction in the films. This would point to the conclusion that the material contains a high crystalline fraction with an amorphous silicon tissue located in the grain boundaries.

4. CONCLUSION

We have reported in this paper a Monte Carlo simulation in order to study the influence of different parameters of a heterogeneous material (especially nanocrystalline or polymorphous silicon thin films) on the evolution of its optical absorption mainly in the infrared spectral region. The results issue from this simulation point to the conclusion that $\alpha_{\text{app}}(E)$ values increase with the decrease of the film thickness mainly in weak energy range. This enhanced optical absorption is due to surface light scattering phenomena which have a vital importance for efficient thin film silicon solar cells.

Acknowledgements: Thanks to all who contributed to this work.

REFERENCES
