THIN FILM SOLAR CELLS AND THEIR OPTICAL PROPERTIES

S. Jurečka[a], E. Pinčík [b], R. Brunner [b]

[a] *DEF FEE UZ, kpt. Nálepku 1390, 03101 L. Mikuláš, Slovakia*
[b] *IoP SAS, Dúbravská cesta 9, 84511 Bratislava, Slovakia*
e-mail: jurecka@lm.utc.sk

Summary In this work we report on the optical parameters of the semiconductor thin film for solar cell applications determination. The method is based on the dynamical modeling of the spectral reflectance function combined with the stochastic optimization of the initial reflectance model estimation. The spectral dependency of the thin film optical parameters computations is based on the optical transitions modeling. The combination of the dynamical modeling and the stochastic optimization of the initial theoretical model estimation enable comfortable analysis of the spectral dependencies of the optical parameters and incorporation of the microstructure effects on the solar cell properties. The results of the optical parameters of the i-a-Si thin film determination are presented.

1. INTRODUCTION

A typical semiconductor solar cell consists of a large-area p-n junction, which is exposed to the light. A certain portion of the radiation energy is absorbed in the device structure and converted into electrical energy, exploiting a physical process known as photovoltaic effect. Solar cells can be made from various semiconductor materials; silicon is widely used today for its low cost. There are two basic types of solid silicon, amorphous (having no long-range order) and crystalline (where the atoms are arranged in an ordered crystal lattice). There are various other terms for the crystalline structure of silicon; polycrystalline, microcrystalline, nanocrystalline etc, and these refer to the size of the crystal grains. The photon can pass through the semiconductor structure or if the photon energy is greater than the bandgap energy it can be absorbed. Absorbed photon excites the valence electron into the conduction band. The absorption process thus creates electron-hole pairs, which diffuse in the solar cell structure. The solar frequency spectrum approximates a black body spectrum at ~6000 K, and the photons energies are greater than the band gap of silicon. These higher energy photons are absorbed by the solar cell, but the difference in energy between these photons and the silicon band gap is converted into heat via the lattice vibrations.

In order to limit the production cost of solar cell as low as possible polycrystalline and amorphous silicon in the thin film structure are used. Polycrystalline structure gives efficiency around 15%. The amorphous silicon is the cheapest and it gives efficiency close to 15%. Amorphous silicon also has a very high optical absorption coefficient, so most of the sunlight is absorbed within approximately 1μ of the amorphous layer surface. The simple structure of thin film amorphous silicon solar cell consists of ultra thin p-type top layer, a thicker intrinsic layer and a very thin n-type bottom layer. The top p-layer is relatively transparent and so most incident light pass right through it to generate free electron-hole pairs in the intrinsic layer. The p and n layers create an electric field across the entire intrinsic region to induce free electric charge movement in the layer.

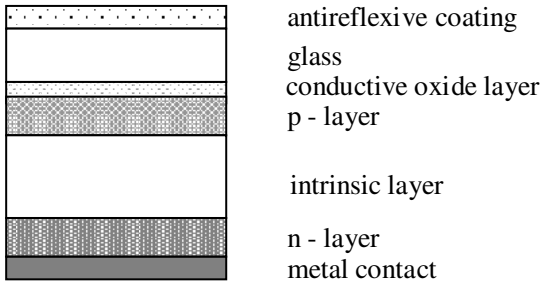

Fig. 1.: Amorphous silicon solar cell structure in a p-i-n design

Optical properties of the amorphous thin film solar cell are important for the conversion efficiency. There are several important features in the structure of the amorphous silicon that influence the optical properties – short-range order, long-range order, and the coordination defects. The coordination defects feature is the most important because it determines the trapping and the recombination of the electronic properties. The electronic structure of amorphous silicon comprised the bands, the band tails, and the defect states in the gap. There exist the tails of states in the conduction and valence bands due to fluctuations of the bond lengths and bond angles in the amorphous silicon matrix. To terminate the dangling bonds, remove the gap states associated with the native defects of amorphous silicon and to build stronger covalent bonds the hydrogenization process creating Si:H bonds is often used. Hydrogen opens up the weak long Si:Si bonds placing as their substitute two stronger Si:H bonds. Recently the cyanidization process is applied to the thin film solar cell structure treatment in order to improve structural, electrical and optical properties [1].

2. DETERMINATION OF THE OPTICAL PARAMETERS OF THE THIN SEMICONDUCTOR FILM

Optical properties of solids can be characterized by the complex index of refraction as a function of photon energy $n(\omega) = \eta(\omega) + i\kappa(\omega)$. Index of refraction provides information on the propagation of radiation and on the electronic structure of solids. The refractive index $\eta(\omega)$ and the extinction coefficient $\kappa(\omega)$ are commonly determined by reflective and absorptive spectroscopies in wide range of photon energies. Theoretical formulations of η and κ can be obtained by the energy-dependent dielectric function derived by the quantum theory for the interaction between radiation and matter considering interband semiconductor transitions. In the experiment the refractive index and the extinction coefficient are measured rather than the dielectric function.

Analytical expressions for the refractive index $\eta(\omega)$ and the extinction coefficient $\kappa(\omega)$ are useful in the determination of fitting parameters and in the analysis of experimentally accesible data. The extinction coefficient can be analytically expressed for semiconductors and insulators by

$$\kappa(\omega) = \frac{\pi f_0}{4\omega_0}\delta(\omega-\omega_0), \qquad (1)$$

where f_0 is the dipole oscillator strength of the transition, ω_0 is the transition energy and δ is the Dirac δ function [2]. In order to satisfy the symmetry relation $\kappa(\omega) = -\kappa(-\omega)$ the extinction coefficient can be transformed into

$$\kappa(\omega) = \frac{\pi f_0}{4\omega_0}[\delta(\omega-\omega_0) - \delta(\omega+\omega_0)]. \qquad (2)$$

This equation assumes the infinite lifetime for the excited state in the transition. In reality the spontaneous emission produces the damping of excited states and the δ functions can therefore be replaced by the Lorentzian function. The extinction coefficient then becomes

$$\kappa(\omega) = \frac{f_0\Gamma_0\omega}{[(\omega-\omega_0)^2+\Gamma_0^2][(\omega+\omega_0)^2+\Gamma_0^2]}, \qquad (3)$$

where Γ_0 is parameter of the Lorentzian function. The refractive index is connected to the extinction coefficient by Kramers - Kronig dispersion relations and can be expressed by

$$\eta(\omega) = \eta_b - \frac{1}{2}\frac{f_0(\omega^2-\omega_0^2-\Gamma_0^2)}{[(\omega-\omega_0)^2+\Gamma_0^2][(\omega+\omega_0)^2+\Gamma_0^2]}, \qquad (4)$$

where η_b is the background refractive index due to the contribution from electrons in inner shells. The above formulations are valid for a single transition of electrons from the valence to the conduction bands. Each transition makes an independent contribution to the extinction coefficient. To express the extinction coefficient for several transitions one can divide the oscillator strength into fractions f_i with transition energy ω_i and Lorentzian coefficient Γ_i. The extinction coefficient and refractive index are then expressed by the sum

$$\begin{aligned}\kappa(\omega) &= \sum_i \kappa_i(\omega,\omega_i,f_i,\Gamma_i),\\ \eta(\omega) &= \sum_i \eta_i(\omega,\omega_i,f_i,\Gamma_i).\end{aligned} \qquad (5)$$

Equations (5) were used for the theoretical spectral reflectance of the thin intrinsic a-Si film model construction. Theoretical and experimental spectral reflectance can then be matched by fitting for the film thickness and optical parameters functions properties. In this work the dynamical modeling and stochastic optimization method (DMSO) was used for the purposes of the thin film optical parameters extraction. The DMSO method was introduced in [3]. The initial theoretical model of the spectral reflectance function is constructed in the DMSO method in the visual graphical environment and enables intuitive estimation of the thin film spectral reflectance function *R* parameters

$$R = \frac{A + Bx + Cx^2}{D + Ex + Fx^2}. \qquad (6)$$

In this equation $x = \exp(-\alpha d)$ is the absorbance, $\alpha = (4\pi\kappa)/\lambda$ is the absorption coefficient and

$A = [(1-\eta)^2+\kappa^2][(\eta+\eta_s)^2+(\kappa+\kappa_s)^2]$
$B = 2[A'\cos\varphi + B'\sin\varphi]$
$C = [(1+\eta)^2+\kappa^2][(\eta-\eta_s)^2+(\kappa-\kappa_s)^2]$
$D = [(1+\eta)^2+\kappa^2][(\eta+\eta_s)^2+(\eta+\kappa_s)^2]$
$E = 2[C'\cos\varphi + D'\sin\varphi]$
$F = [(1-\eta)^2+\kappa^2][(\eta-\eta_s)^2+(\kappa-\kappa_s)^2]$
$A' = (1-\eta^2-\kappa^2)(\eta^2-\eta_s{}^2+\kappa^2-\kappa_s{}^2)+4\kappa(\eta\kappa_s-\eta_s\kappa)$
$B' = 2(-\eta^2-\kappa^2)(\eta\kappa_s-\eta_s\kappa)-2\kappa(\eta^2-\eta_s{}^2+\kappa^2-\kappa_s{}^2)$
$C' = (1-\eta^2-\kappa^2)(\eta^2\eta_s{}^2\kappa^2-\kappa_s{}^2)-4\kappa(\eta\kappa_s-\eta_s\kappa)$
$D' = 2(1-\eta^2-\kappa^2)(\eta\kappa_s-\eta_s\kappa)+2\kappa(\eta^2-\eta_s{}^2+\kappa^2-\kappa_s{}^2)$
$\varphi = (4\pi\eta d)/\lambda$ [4].

In these equations index *s* denotes the substrate characteristics and *d* is the film thickness. In the extinction coefficient and refractive index functions (5) ten optical transitions were accounted. The spectral reflectance function (6) then contains 32 independent variables. In the next step the initial spectral reflectance function was refined by the genetic algorithm method and by the combination of traditional numerical optimization methods (Nelder - Mead downhill simplex and Marquardt - Levenberg method).

3. EXPERIMENTAL RESULTS

Experimental spectral reflectance data of the i-a-Si thin film were analyzed. Thin i-a-Si film sample was deposited at the Osaka University, Japan, on Corning 1737 glass substrate by the CVD method. The spectral reflectance of the film was measured in the near normal incidence geometry in the spectral region 215 – 900 nm (Fig. 2).

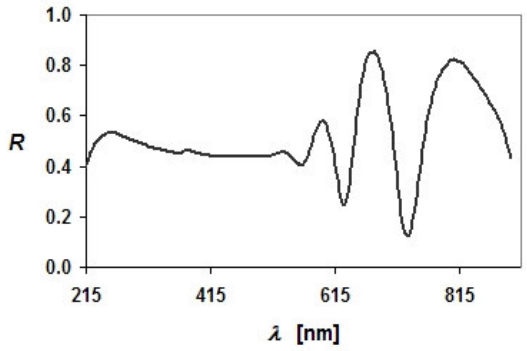

Fig. 2. Spectral reflectance R of the thin i-a-Si film on glass substrate

The refractive index and the extinction coefficient spectral dependencies in the near UV and VIS regions were determined by the DMSO method with the dispersive model (5) (Fig. 3 and Fig. 4).

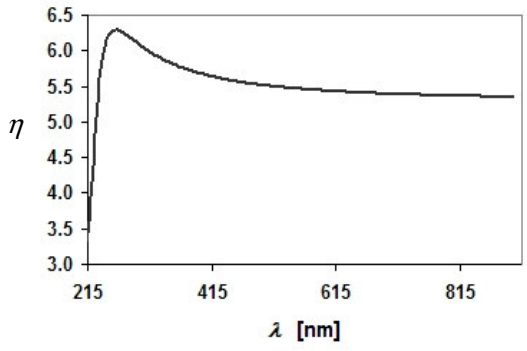

Fig. 3. Refractive index of the thin i-a-Si film determined by the DMSO method

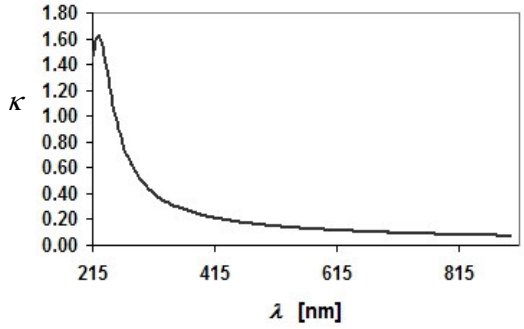

Fig. 4. Extinction coefficient of the thin i-a-Si film determined by the DMSO method

DMSO method based on dispersive relations (5) succeeded in theoretical reflectance model refinement very good. It does not converge to a local optimum of the refined model. The combination of dynamical modeling and stochastic optimization of the initial mathematical model compared with the experimental data speeds up calculations and gives meaningful optical parameters. Implementation of the visual modeling and genetic algorithm optimization method enables building up the thin film microstructure constraints into the optical parameters dispersion model and optimize the solar cell structure design.

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