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Analysis And Optimization Of Multilayer Silicon Structures Via Ellipsometry For Solar Cell Efficiency

Soliyev O.M.
Andijan State University, Uzbekistan

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Abstract: This study presents a comprehensive analysis of multilayer silicon-based structures using spectroscopic ellipsometry to enhance the performance of solar cells. By measuring ellipsometric parameters (Ψ and Δ) across a wide spectral range and applying effective medium approximations, the optical properties of monocrystalline (c-Si), polycrystalline (pc-Si), and amorphous silicon (a-Si) layers are thoroughly investigated. The research incorporates numerical modeling, structural reconstruction, and cross-sectional transmission electron microscopy (XTEM) to validate layer thickness, composition, and surface morphology. The results highlight the impact of grain boundaries, surface roughness, and void fractions on light absorption and penetration depth, particularly in the short-wavelength region. The proposed methodology enables accurate characterization and optimization of thin-film structures, contributing to improved solar energy conversion efficiency.

Keywords: Spectroscopic ellipsometry, polycrystalline silicon, multilayer structures, optical characterization, effective medium approximation, solar cells, thin films, light penetration depth, transmission electron microscopy, photovoltaic efficiency.

INTRODUCTION:

Ellipsometry is a method that allows determining the optical parameters of multilayer systems with high precision [1]. By measuring the ellipsometric angles Ψ and Δ and performing subsequent modeling, it is possible to obtain important information about the structure and properties of the investigated materials, such as polycrystalline silicon.

Ellipsometry measures changes in the polarization of light upon its reflection from or transmission through a material [2]. The two main parameters measured in ellipsometry are Ψ and Δ, which describe the change in amplitude and phase of the polarized components of light, respectively. These parameters depend on the thickness of the layers, the refractive indices, and the extinction coefficients of the materials in the studied system.

The method is non-destructive and can be applied to both transparent and absorbing layers over a wide spectral range. Because of this, ellipsometry is widely used in microelectronics, nanotechnology, photonics, and in quality control of thin films.

2. LITERATURE REVIEW

The ellipsometry method is based on changes in the polarization state of light upon its reflection from a surface. By defining the polarization state before reflection from a sample and measuring it after reflection, one can obtain information about the reflecting surface. The main measured parameters are Ψ and Δ: Ψ describes the change in the amplitude of polarized light, while Δ represents the phase shift of the polarized light. These parameters are related to the complex reflection coefficient ρ, which is defined as the ratio of the reflection coefficients for the parallel (r_p) and perpendicular (r_s) polarization components:

$$\rho = \frac{r_p}{r_s} = tg(\Psi)e^{i\Delta}$$

The main goal of ellipsometry is to determine the optical parameters of the system, such as the refractive index (n), extinction coefficient (k), and layer thickness, provided that the experimental values of the ellipsometric angles Ψ and Δ are known [3].

If a film consists of a mixture of several components, the effective medium approximation is often used to analyze its optical properties. This approximation assumes that the behavior of light in a multilayer structure can be described as light propagation in a homogeneous medium with certain effective optical parameters, which account for the contributions of each component according to their volume fractions or other characteristics.

To determine the effective parameters, various theoretical models can be applied, such as the Lorentz or Drude models for the dielectric function of materials, as well as more advanced approaches like the Bruggeman or Maxwell-Garnett models, which take into account microstructural features [4].

It should be noted that in recent decades spectroscopic ellipsometry has become increasingly widespread, as it enables the measurement of Ψ and Δ over a broad spectral range. This makes it possible to more accurately reconstruct optical parameters, determine the composition, thickness, and inhomogeneity of thin films, which is particularly important for microelectronics, nanotechnology, and photonics.

Let us assume that a multilayer film consists of two materials: a dielectric with refractive index n_1 and a metallic layer with refractive index n_2. Based on the volume fractions f_1 and f_2 of these components, the effective optical parameters can be estimated.

Effective refractive index:

$$n_{eff} = f_1 \cdot n_1 + f_2 \cdot n_2$$

Effective absorption coefficient:

$$k_{eff} = f_1 \cdot k_1 + f_2 \cdot k_2$$

where k_1 and k_2 are the absorption coefficients of each component, respectively [5].

This linear approximation is the simplest approach to describe mixtures. However, in practical applications, more sophisticated effective medium models are often employed, such as the Maxwell–Garnett or Bruggeman approximations, which take into account the interaction of electromagnetic waves with the microstructure of the material.

3. RESEARCH METHODOLOGY

In this work, the following research methods were applied: measurements using a spectral ellipsometer; acquisition of ellipsometric data in the visible spectral range at different wavelengths; processing of the obtained ellipsometric data taking into account the dependence on the probing radiation penetration depth; construction of multilayer structure models including layer parameters such as thickness, refractive index, and extinction coefficient; application of the least-squares method to fit theoretical curves to the experimental data.

4. Results and Discussion

The modeling and interpretation of ellipsometric data were carried out in several stages:

– performing spectral ellipsometry to measure the ellipsometric angles Ψ and Δ at different wavelengths and angles of incidence;

– constructing an initial structural model using known optical parameters and layer thicknesses;

– incorporating physically justified assumptions about the behavior of light upon reflection from a multilayer structure.

To model the mixture of amorphous and crystalline silicon with voids, the effective medium approximation (EMA) was applied. Within this approach, the mixture is considered as a homogeneous medium with effective optical parameters that depend on the volume fractions of its components.

The refractive index and absorption coefficient of amorphous silicon are denoted as:

$$n_{a-Si}(\lambda), \qquad k_{a-Si}(\lambda)$$

For crystalline silicon:

$$n_{c-Si}(\lambda), \qquad k_{c-Si}(\lambda)$$

For voids:

$$n_{void} = 1, \qquad k_{void} = 0$$

The effective refractive index neff(λ) and absorption coefficient keff(λ) are calculated based on the volume fractions and optical parameters of the components.

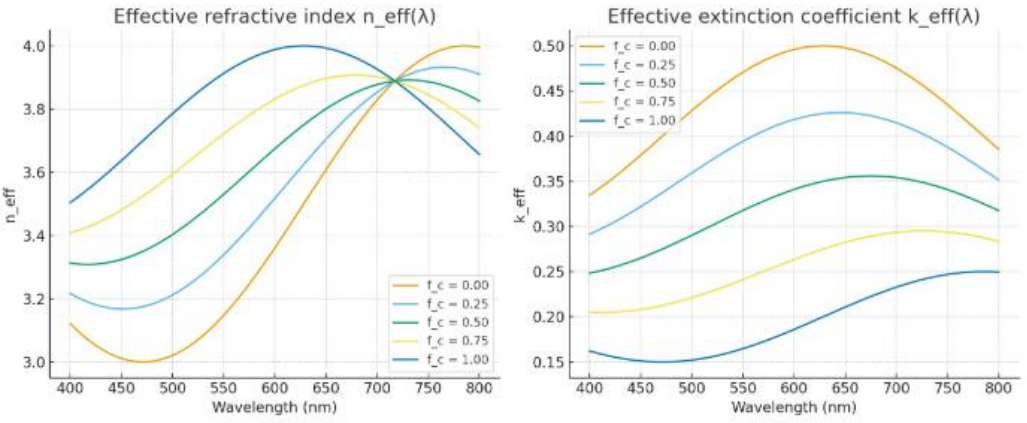

Fig.1. The effective refractive index n_eff (λ) and absorption coefficient k_eff (λ).

The effective refractive index n_eff (λ) is plotted as a function of different values of f_c (the crystalline silicon fraction). As the crystalline silicon fraction increases, the value of n_eff also increases (Fig.1. a).

The effective extinction coefficient k_eff (λ) is shown for different values of f_c.Here, k_eff represents the absorption of light, and with an increasing crystalline phase fraction, stronger absorption is observed (Fig.1. b).

For the investigation of polycrystalline silicon (pc-Si), spectral ellipsometry was combined with cross-section transmission electron microscopy (XTEM). These methods complement each other, providing comprehensive information about the structure and properties of the material [6].

Additionally, comparison of the ellipsometric modeling results with XTEM images allows for validation of the derived structural parameters such as grain size, layer thickness, and porosity. This combined approach ensures a higher accuracy in determining the optical constants of pc-Si and reveals correlations between microstructural features and optical behavior. Such integrated analysis is especially important for applications in thin-film photovoltaics, where the balance between crystallinity, void fraction, and absorption strongly influences device efficiency.

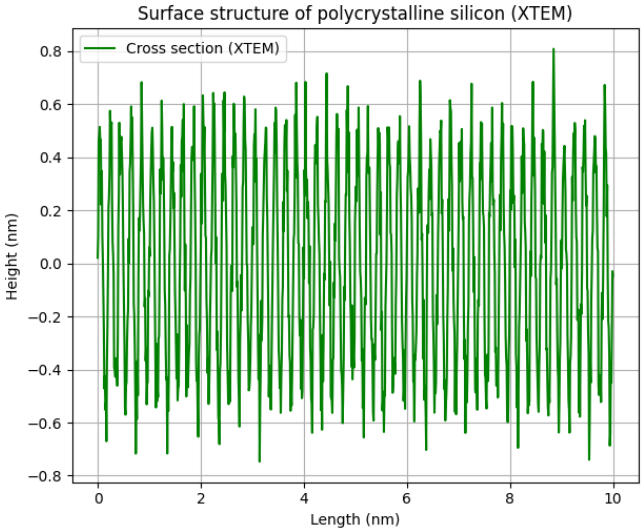

Fig. 2. Surface structure of polycrystalline silicon (XTEM)

Fig.2 shows the details of the microstructure of the surface layer of the polycrystalline Si film in the studied system. The grain size of the polycrystalline silicon film is approximately 100 Å. The technologically fabricated structure consisted of a crystalline silicon substrate (c-Si), a silicon dioxide layer (SiO2), and a polycrystalline silicon film (pc-Si).

Cross-sectional transmission electron microscopy (XTEM) revealed important structural details of the h-c-Si/SiO_2/pc-Si system.

Analysis of ellipsometric spectra provides valuable quantitative information about the composition and thickness of the different layers in the studied system [7], [8]. Figures 3(a) and 3(b) show the experimental

and calculated Ψ and Δ spectra (for an incidence angle of 70°) of the investigated structure. It can be observed that the spectra differ not only quantitatively but also qualitatively. This may indicate the need for a more accurate model of the structure, taking into account additional factors such as surface roughness and thickness inhomogeneity, as previously mentioned.

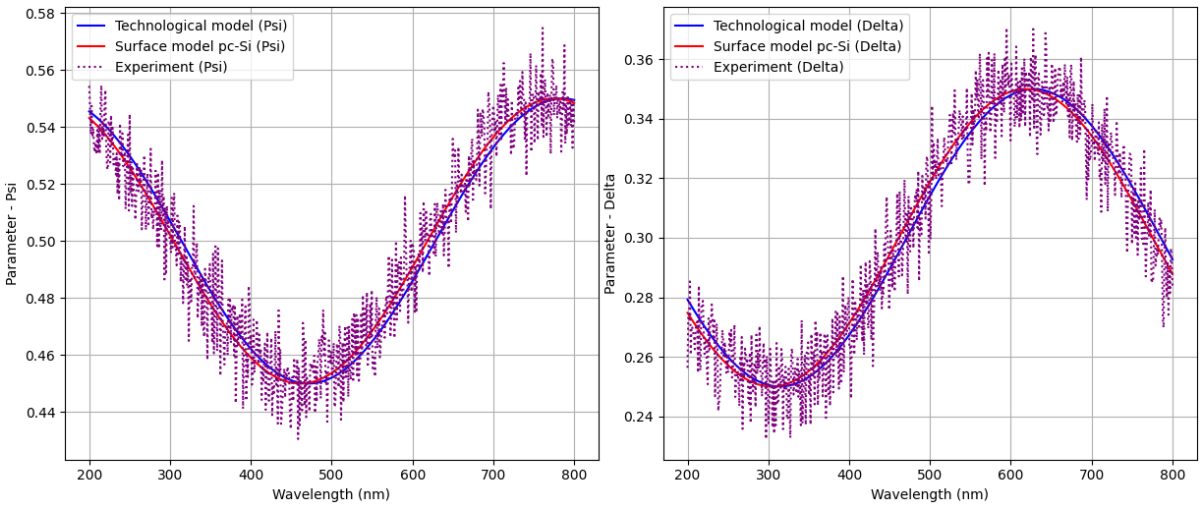

Fig.3. a) Spectra of ellipsometric parameters (Psi); b) Spectra of ellipsometric parameters (Delta).

The observation that spectra 1 and 2 coincide at λ < 400 nm suggests that for wavelengths below 400 nm, both the technological model and the pc-Si surface model provide equivalent optical characteristics. This implies that in this wavelength range, these models adequately describe the optical properties of the material.

The study also shows that microstructural parameters, such as grain size distribution, interfacial diffusion, and the presence of voids, can significantly affect the ellipsometric spectra. Therefore, modeling of experimental data should consider not only the average thickness and optical parameters of the layers but also such uncertainties. This approach allows for a more precise optical characterization of the structure, which is crucial for evaluating the performance of optoelectronic devices.

The coincidence of the ellipsometric parameter spectra at λ < 400 nm confirms that, in this wavelength range, both the technological model and the surface model of pc-Si accurately describe the optical properties of the material. Experimental data may slightly deviate due to various factors, such as surface inhomogeneities or measurement accuracy; however, overall, they should align well with theoretical models.

To unambiguously determine the actual structure model of h-c-Si/SiO_2/pc-Si, we relied on physically grounded considerations and results obtained using cross-sectional transmission electron microscopy. This approach enabled more accurate modeling and analysis of the structure.

Analysis of the penetration depth spectra of the probing radiation into various forms of silicon (monocrystalline c-Si, polycrystalline pc-Si, and amorphous a-Si) allows for a better understanding of how different structures absorb and convert solar energy. Depending on the crystalline structure, silicon has different optical properties that affect the depth of light penetration and energy conversion efficiency [9].

Due to the presence of grain boundaries and other defects in polycrystalline silicon, light penetrates the material to a shallower depth compared to monocrystalline silicon. This limits its efficiency in the near-infrared region, but it still allows for effective absorption of visible light [10].

The penetration depth spectra of probing radiation in different types of silicon-such as monocrystalline (c-Si), polycrystalline (pc-Si), and amorphous (a-Si)-are crucial for understanding their optical and photoelectric properties. These spectra show how deeply light of various wavelengths penetrates into the materials and how effectively they can absorb and convert solar energy.

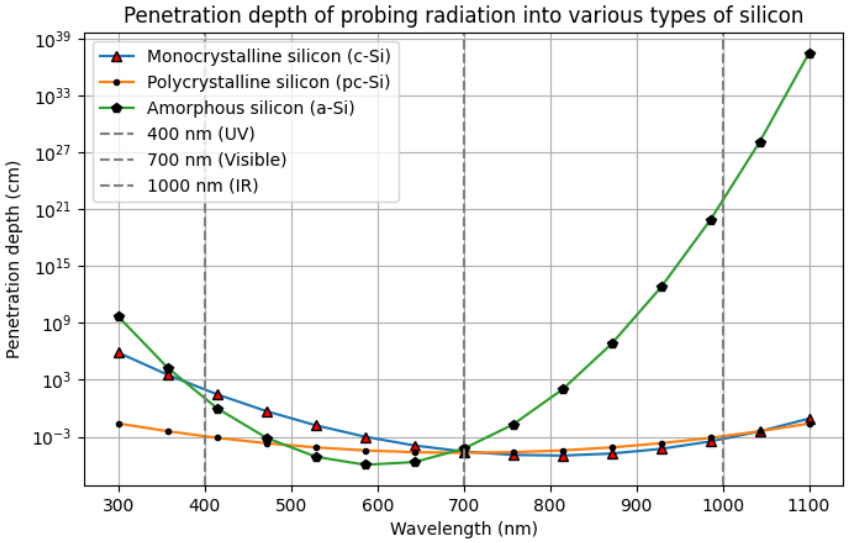

Fig.4. Penetration depth of probing radiation in various types of silicon

As seen in Fig. 4, monocrystalline silicon (c-Si) exhibits a greater penetration depth in the near-infrared range (> 800 nm), indicating efficient absorption of long-wavelength light. Polycrystalline silicon (pc-Si) has a shallower penetration depth compared to monocrystalline silicon, especially in the visible and infrared ranges. Amorphous silicon (a-Si) shows a very small penetration depth, making it effective for absorbing short-wavelength light (<600 nm), but less efficient for long-wavelength light.

Modeling and experimental data show that for wavelengths below 400 nm, the sensitivity depth of the technological system is less than 200 nm. This means that at these wavelengths, interference effects within the bulk of the material are less significant, and light does not penetrate deeper than 200 nm. This is important to consider when designing and analyzing thin-film structures and technological systems based on polycrystalline silicon.

5. CONCLUSION

The analysis of radiation in the silicon system and the development of effective models of the multilayer surface structure are based on an understanding of the optical properties of materials, interference effects, and the processes of absorption and charge carrier recombination. The use of matrix modeling methods and numerical techniques allows for the optimization of multilayer structures to improve the efficiency of solar cells. A comprehensive approach to modeling and optimizing such systems enables significant enhancement of their performance and broadens their application scope.

The study of the polycrystalline silicon surface requires consideration of various factors such as grain boundaries, surface roughness, and impurities in order to accurately describe the experimental data. The use of more advanced models that incorporate these factors allows for better alignment with the experimental spectra, especially in the short-wavelength region. This contributes to a more accurate characterization of the material and improvement of its optical properties for use in photovoltaic devices.

REFERENCES

Rzhanov, A. V., & Ilyin, L. A. (Eds.). (2009). Ellipsometry: Theory, methods, applications (192 p.). Nauka. [in Rus.]

Fujiwara, H. (2007). Spectroscopic ellipsometry: Principles and applications. John Wiley & Sons.

Tompkins, H. G., & Irene, E. A. (Eds.). (2005). Handbook of ellipsometry. William Andrew Publishing.

Rzhanov, A. V. (Ed.). (2007). Ellipsometry – A method for surface investigation (180 p.). Nauka. [in Rus.]

Jellison, G. E., & Modine, F. A. (2016). Parameterization of the optical functions of amorphous materials in the interband region. Applied Physics Letters, 69(3), 371–373. (https://doi.org/10.1063/1.118064)

Shvets, V. A., et al. (2009). Ellipsometry – A precision method for monitoring thin-film structures with sub-nanometer resolution. Russian Nanotechnology, 4 (3–4), 72–83. [in Rus.]

Prokopenko, V. T., et al. (2018). Ellipsometry of optical compounds of optoelectronic element materials. Izvestiya Vysshikh Uchebnykh Zavedenii. Instrument Engineering, 51(10). [in Rus.]

Shokhovets, S., Fabel, B., Kranz, L., & Lux-Steiner, M. C. (2010). Optical properties of polycrystalline silicon films characterized by spectroscopic ellipsometry and transmission electron microscopy. Thin Solid Films,

518 (22), 6381–6385. (https://doi.org/10.1016/j.tsf.2010.06.064)

Alonso, M. I., Garriga, M., Tobías, I., & Morante, J. R. (2003). Optical functions of hydrogenated amorphous silicon: Effect of deposition temperature. Journal of Applied Physics, 94 (1), 611–617. (https://doi.org/10.1063/1.1577406)

Khashim, K., et al. (2017). Application of spectroscopic ellipsometry for the characterization of nanoscale films. Physics of the Solid State, 59(11), 2191–2195. [in Rus.]

Ghita, B. V., Florea, S., Mihaila, M., & Brinza, F. (2014). Analysis of light absorption in thin-film solar cells using spectroscopic ellipsometry. Solar Energy, 107, 757–765. (https://doi.org/10.1016/j.solener.2014.06.022)