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Optical and Structural Properties of CdTe Thin Films for Photovoltaic Applications

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The paper presents the results of a study of cadmium telluride thin films grown on glass substrates by open evaporation in vacuum. Based on experimentally measured optical transmittance spectra of the films, their optical parameters were calculated using the OPTIFIT software environment. A comparative analysis of the film thickness measured with a profilometer and the OPTIFIT model showed only minor deviations in thickness for thin films up to 3-4 µm. Analysis of AFM images revealed a significant improvement in the structural characteristics of CdTe films, in particular a reduction in the number of defects and in surface roughness for thicknesses of 500–2500 nm, which contributes to increasing the efficiency of photovoltaic energy converters.

Keywords: renewable energy, thin-films, CdTe, solar cell, optical properties, OPTIFIT, software, computer simulation, semiconductors.

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Introduction

The conversion of solar energy using photovoltaic installations plays a significant role in meeting increasing energy needs, particularly given the gradual depletion of conventional energy resources. The conversion of solar radiation into electricity occurs without the processes typical of conventional power generation; therefore, photovoltaic (PV) systems do not produce direct emissions or other pollutants, and the environmental burden is largely confined to the manufacturing and end-of-life management stages of the components. Within the field of photovoltaic conversion, substantial attention has been focused on second-generation solar cells, especially cadmium telluride (CdTe)-based devices [1]. Cadmium telluride is one of the most widely studied semiconductor materials for photovoltaic devices, owing to its near-optimal bandgap, strong optical absorption, and compatibility with a wide range of deposition methods [2,3]. Thin films can be deposited using both physical methods (vacuum evaporation, magnetron sputtering, etc.) and chemical methods (chemical bath deposition (CBD), electrochemical deposition, and chemical vapor deposition (CVD)), each of which yields films with distinct structural and optical properties. Therefore, research on the microstructure and optical properties of CdTe thin films is of importance for further improving solar-cell efficiency, since the optical characteristics are directly related to the performance of solar cells.

I. Literature Review and Problem Statement

The authors of publication [4] report a study of the optical, electronic, and structural properties of cadmium telluride (CdTe) thin films deposited by thermal evaporation on glass substrates. X-ray diffraction (XRD) analysis revealed that the CdTe film is polycrystalline, exhibiting a diffraction peak at $2\theta = 23.61°$, which corresponds to the zinc blende structure with a preferred orientation along the (111) plane. The lattice parameter was found to be $a = 6.529$ Å, and the bandgap energy was 1.534 eV. The modeling results indicated that the local density approximation (LDA) substantially underestimates the bandgap and the energy levels of the Cd 4d states, and it also fails to describe the s-d coupling accurately; however, it reproduces the spin-orbit interaction correctly. The use of the LDA+U approach (local density approximation with a Hubbard U parameter) enabled correction of the Cd 4d level positions and split a single *s* peak into two, which is consistent with experimental photoemission data and indicates significant s-d hybridization. Optical spectra (absorption and reflectance coefficients, as well as the refractive index) calculated using LDA and LDA+U showed good agreement with experiment after applying a scissors operator to correct the bandgap, although some deviations were observed in the magnitudes of the absorption and reflectance peaks.

In study [5], the optical properties of CdTe thin films deposited on glass/ITO substrates by radio-frequency (RF) magnetron sputtering were investigated. The aim was to determine the optical constants (refractive index, absorption coefficient, and extinction coefficient) as well as the film thickness based on an analysis of the transmittance spectrum using the envelope method. Two films with deposition times of 0.5 and 1.25 h were examined, yielding thicknesses of 1.393 µm and 3,200 µm, respectively. The presence of well-defined interference maxima and minima in the spectra indicated high film quality. The refractive index exhibited normal dispersion, decreasing with increasing wavelength. The bandgap energy, determined from the Tauc plot $(ahv)^2$ as a function of hv, was 1.42 eV and 1.44 eV for the two samples, which is in good agreement with literature values.

Study [6] focuses on the effect of substrate temperature on the microstructure, morphology, and the optical and luminescent properties of CdTe thin films deposited on glass substrates by close-spaced sublimation (CSS). The results indicate that growth temperature significantly affects film quality: increasing the temperature leads to larger grain size, improved crystallinity, and reduced, with an optimum temperature of approximately 540°C. Optical measurements revealed a shift of the absorption edge and an increase in the bandgap with temperature, while photoluminescence spectroscopy was used to investigate the origin of luminescence peaks associated with the band edge, structural defects, and surface states. The study demonstrates that the CSS method enables the fabrication of high-quality CdTe films with strong potential for application in photovoltaic solar cells.

The publication [7] reports the results of a study on CdTe thin films prepared by electrodeposition of FTO-coated glass substrates, followed by annealing in air at 200-450°C. X-ray diffraction (XRD) results show that the as-deposited films have a nanocrystalline cubic structure with a grain size of about 6 nm, whereas heat treatment leads to grain growth and the formation of polycrystalline films. Optical measurements revealed a nonlinear dependence of the bandgap energy on the annealing temperature: it decreased from 1.48 eV to 1.45 eV at 300°C and the increased again at 450°C. Based on these films, a solar cell with an open-circuit voltage of 500 mV and short-circuit current density of 1.2 mA/cm^2 was fabricated, confirming the potential of CdTe for photovoltaic applications.

A review of the published papers indicates that limited attention has been paid to investigating the effect of deposition parameters on the structure and optical properties of CdTe thin films of varying thickness, particularly in photovoltaic applications.

The aim of this work is to experimentally study a series of CdTe samples of varying thickness deposited by thermal evaporation on glass substrates, to investigate the influence of surface morphology on optical transmittance spectra, and to determine the optical properties of the films using computer simulation methods.

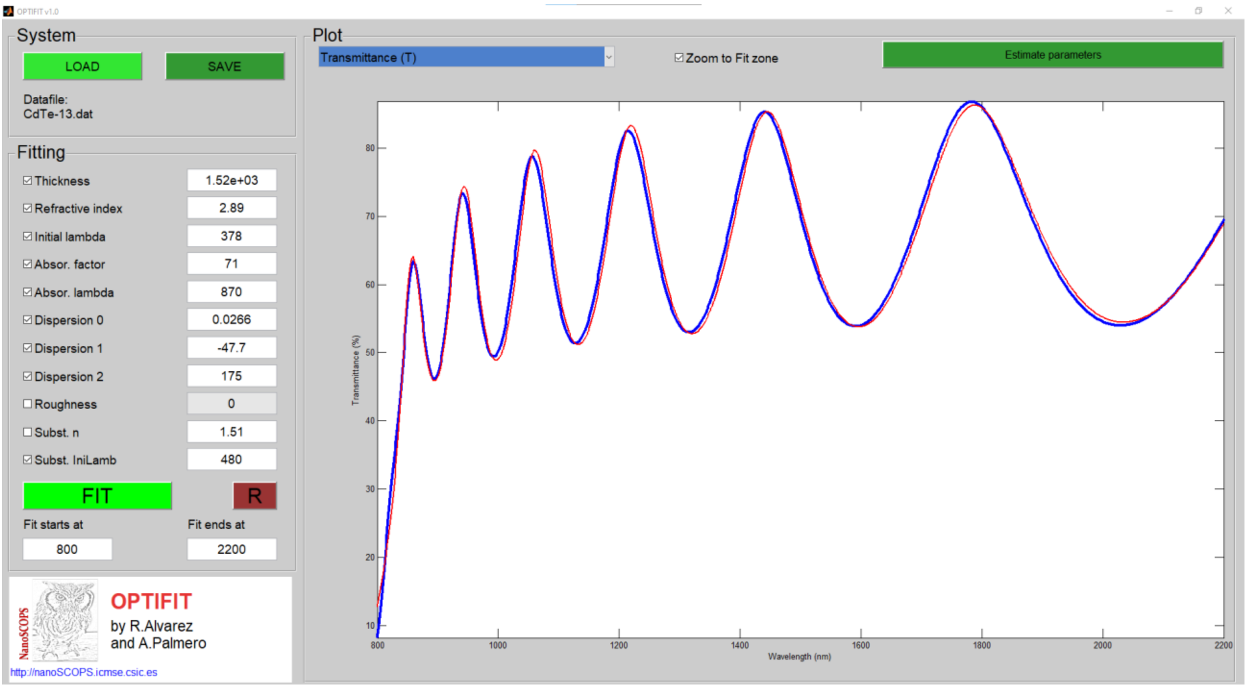
II. Methods

Thin films of cadmium telluride on 0.17-mm-thick glass substrates were obtained using a low-cost method – open-vacuum evaporation from synthesized Cd–Te compounds. During deposition, the substrate temperature was T_{sub} = 475 K. The film thickness was controlled by the deposition time, which ranged from 120 to 570 s. The deposition conditions were characterized by the CdTe evaporation temperature T_{evap} = 790-850 K, which ensured an optimal sublimation rate.

The optical transmission spectra for the obtained films were measured using an Agilent Technologies Cary Series UV-Vis-NIR spectrophotometer in the range of 500-2500 nm.

The use of atomic force microscopy (AFM), which operates on the principle of detecting van der Waals force interactions between the probe tip and the film surface by recording the deflection of an elastic cantilever using a laser optical system and enabling visualization of the surface morphology as well as determination of the sample roughness parameters, made it possible to obtain surface images for their subsequent analysis in the Gwyddion software environment. A more detailed description of the AFM surface characterization methodology is given in [8]. Film thickness measurements were performed using a Dektak XTL profilometer.

Analysis of the obtained optical transmittance spectra for CdTe films was performed using the OPTIFIT software package (Optical parameters from transmittance spectrum), Fig. 1, developed at the Science Institute of Seville, Seville (Spain) by the researchers Rafael Alvarez and Alberto Palmero [9]. Based on the measured optical transmittance spectrum, the program allows determination of the film thickness, refractive index, and absorption coefficient. OPTIFIT performs parametric fitting of the measured transmittance spectrum of a thin film on a substrate to a theoretical calculation using established optical models. The mathematical relationship between the transmittance spectrum and the film optical parameters is determined on the basis of the Swanepoel equations [10], which take into account light interference in an absorbing thin film deposited on a transparent substrate. The dispersion of the refractive index is described using the Sellmeier equation, providing a physically consistent and smooth spectral dependence of the refractive index in the transparent region [11]. The extinction coefficient is determined using a model that includes the interband absorption region and a Taylor-series expansion in frequency to account for dispersion outside the absorption edge [12]. The effect of surface roughness on the transmittance spectra is taken into account using the



Datafile:
CdTe-13.dat

☑ Thickness	1.52e+03
☑ Refractive index	2.89
☑ Initial lambda	378
☑ Absor. factor	71
☑ Absor. lambda	870
☑ Dispersion 0	0.0266
☑ Dispersion 1	-47.7
☑ Dispersion 2	175
☐ Roughness	0
☐ Subst. n	1.51
☑ Subst. IniLamb	480

Fit starts at 800
Fit ends at 2200

Transmittance (T)
☑ Zoom to Fit zone

Fig. 1. Graphical user interface of the OPTIFIT software.

approach proposed by Tikhonravov et al. [13]. An initial estimate of the film thickness and refractive index is obtained by the envelope method, as summarized in the review by Poelman and Smet [14].

An advantage of using the OPTIFIT software is the ability to analyze transmittance spectra of relatively thin layers in which a large number of interference extrema are absent. In contrast to classical approaches, in particular the Swanepoel method, the program does not require the presence of three consecutive minima of the transmittance curve T(%) within the investigated spectral range, which significantly expands the possibilities for analyzing the obtained samples. Accordingly, this provides more flexible matching of the experimental data to the calculated curve and increases the informativeness of the analysis.

III. Results and Discussion

To evaluate the optical properties of the thin films, a series of samples was prepared under different deposition conditions, in particular by varying the evaporator temperature and deposition time (table. 1). This made it possible to trace the influence of these parameters on film-structure and film-thickness growth, and to investigate the optical properties of the films.

Table 1.

Experimental parameters of the obtained films

Sample	s.1	s.2	s.3	s.4
Thickness, nm	320	565	1490	7200
T_{sub}, K	475	475	475	475
T_{evap}, K	823	823	790	850
T_{dep}, s	120	150	300	570

For an in-depth analysis of the optical properties, the OPTIFIT software package was used. It performs parametric fitting of transmittance spectra based on the analysis of thin-film interference oscillations and allows determination of the refractive-index dispersion n(λ), the extinction coefficient, and the absorption coefficient, as well as a refined film thickness from the wavelength dependence of transmittance T(λ). The fitting results in the 500–2000 nm spectral range (Table 2) show overall good agreement between the experimentally determined and calculated thicknesses for samples s.2–s.4, whereas for s.1 a certain deviation is observed, which may be attributed to film non-uniformity or an early stage of film formation.

Table 2.

Results of OPTIFIT simulation in the 500-2000 nm range

Parameter	s.1	s.2	s.3	s.4
Thickness, nm	249	591	1490	8790
Refractive index (589 nm)	2.6	2.95	2.94	2.6
Initial lambda, nm	320	385	379	382
Absor. factor	1.7	44.6	86	27.3
Absor. lambda, nm	1040	900	867	860
Subst. n	1.51	1.51	1.51	1.51

The obtained refractive-index values at 589 nm fall within the range n = 2.6–2.95, which is consistent with literature data for polycrystalline CdTe films. The increased n values for samples s.2 and s.3 may indicate improved structural densification and reduced film porosity under the corresponding deposition conditions. The absorption-related parameters (Absor. factor and Absor. lambda) suggest a shift of the fundamental absorption edge to the 860–1040 nm region, which is consistent with the CdTe band-gap energy and possible variations in defect structure depending on the deposition conditions.

The transmittance spectra obtained from the modelling (Fig. 2) exhibit a high degree of overlap between the theoretical and experimental curves for all investigated samples. The clearly pronounced interference maxima and minima, especially for the thicker films (s.3, s.4), confirm the thickness uniformity of the layer and the validity of the applied model. Thus, the OPTIFIT modelling results indicate the adequacy of the chosen approach and the high reliability of the determined optical parameters, enabling a well-founded analysis of how the deposition conditions affect the structural and optical properties of CdTe films.

Figure 2 presents the modelling results of the optical transmittance spectra of CdTe thin films with different thicknesses, obtained by fitting the experimental data using the OPTIFIT program in the 500–2000 nm range. Each plot shows the experimental data points and the theoretical model curve, which makes it possible to assess the degree of agreement.

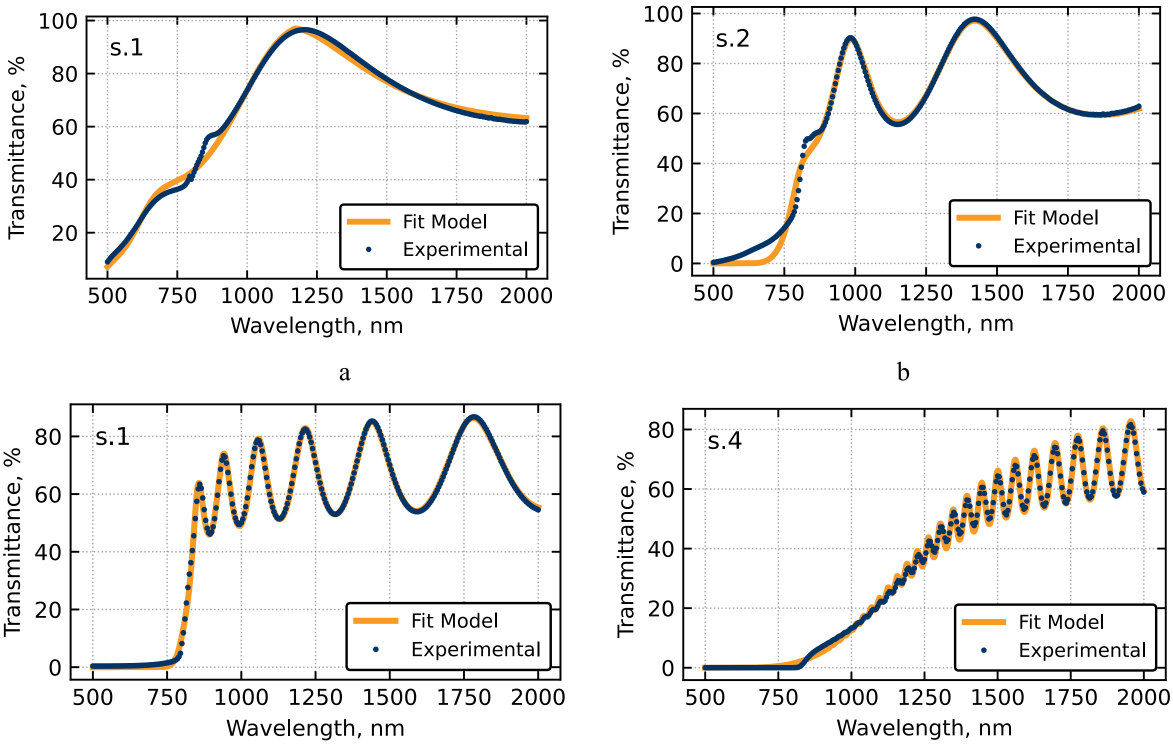
The presented figures show the modelling results of the optical transmittance spectra of CdTe thin films with different thicknesses. As the film thickness increases, a systematic enhancement of interference effects is observed in the transmittance spectra, which is caused by multiple reflections of light at the air–film and film–substrate interfaces. The positions of the maxima and minima are governed by the optical thickness n_d; therefore, increasing the physical thickness leads to a larger number of oscillations within the given spectral range. At wavelengths above ~800 nm, the films exhibit high transparency, indicating a low absorption coefficient in the sub-bandgap region and good structural uniformity. Near the absorption edge, a sharp decrease in transmittance is observed, associated with interband electronic transitions that determine the material band-gap energy. The agreement between the experimental and calculated spectra confirms the adequacy of the interference model and the correctness of the determined optical parameters.

Fig. 3 shows AFM images of the surface morphology of CdTe thin films obtained using atomic force microscopy.

Analysis of the obtained AFM images (Fig. 3) and profilograms (Fig. 4) reveals a characteristic Stranski-Krastanov growth mechanism, in which, at the initial stage, a continuous smooth wetting layer forms on the substrate surface. After the film reaches a critical thickness, a transition to three-dimensional island growth is observed, as evidenced by granular structures. This behavior is caused by the accumulation of strain associated with the lattice-parameter mismatch between the layer and the substrate.

Increasing the film thickness to 500 nm leads to a significant improvement in the surface-structure uniformity; however, with a further increase in thickness beyond 5 µm, grain coarsening and smoothing of the apices of the pyramidal structures are observed.

Based on the analysis of the obtained results, it has been shown that the use of thermal vacuum deposition methods makes it possible to control structural changes during the deposition process, enabling the fabrication of films with predictable optical properties. In particular, an improvement in the structural characteristics of cadmium telluride films is observed, which is reflected in a decrease in the number of defects and a reduction in surface roughness. These positive changes are achieved when the substrate temperature is 475 K, the evaporation temperature is in the range of approximately 788-823 K, and the film thickness is within 500-1500 nm.



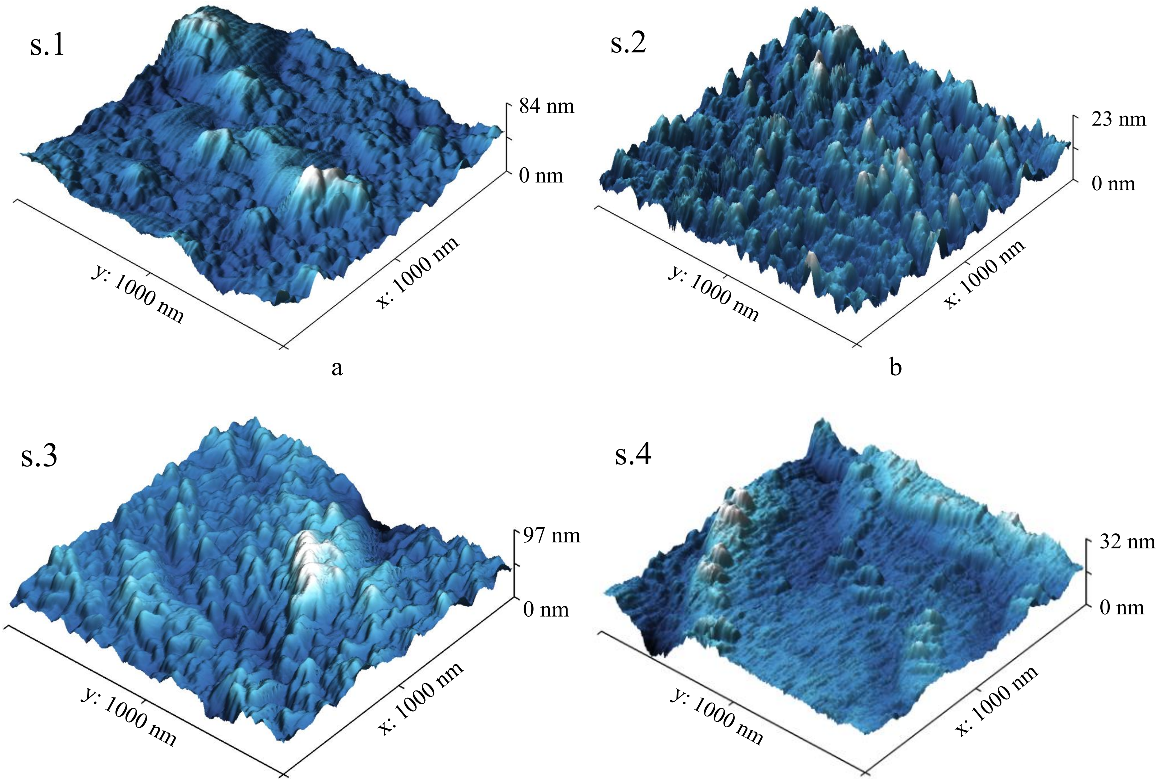
a

b

c

d

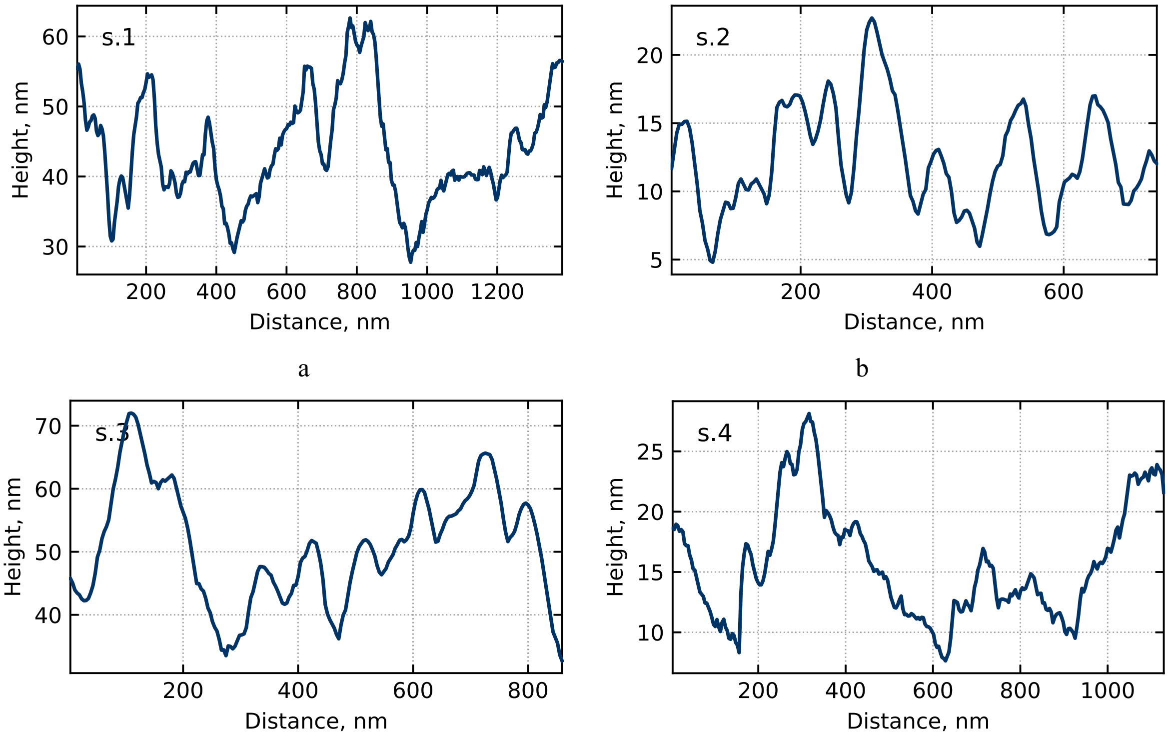
Fig. 2. OPTIFIT simulation results for samples s.1–s.4. a – 249 nm; b – 591 nm; c – 1490 nm; d – 8790 nm.



a b

c d

Fig. 3. Surface morphology of CdTe thin films of different thicknesses obtained by AFM analysis. a – 249 nm; b – 591 nm; c – 1490 nm; d – 8790 nm.



a b

c d

Fig. 4. Surface profilograms of the samples. s.1-s.4 a – 249 nm; b – 591 nm; c – 1490 nm; d – 8790 nm.

Based on the analysis of the optical transmittance spectra, the CdTe thin films deposited on glass substrates exhibit high transmittance in the near-infrared region (λ > 800 nm), reaching ~75–95%, along with a high absorption coefficient in the spectral range approaching the fundamental absorption edge (near the band-gap region). This combination of high transparency and an optimized film thickness (1.5–2.5 μm) indicates that films produced by the present method under the specified technological parameters are suitable for application in thin-film photovoltaic devices based on CdTe/CdS heterostructures.

A comparison of the experimental measurement results with the values calculated using OPTIFIT indicates only minor deviations in the obtained data. This can be attributed to the considerable difficulty of constructing an ideal model of the transmittance spectrum, as well as to increased measurement errors during experimental studies of films with thicknesses exceeding 5 µm.

One of the further ways to increase efficiency may be to introduce alloying impurities into cadmium telluride [15].

Conclusions

Using the open-vacuum evaporation method, a series of CdTe thin-film samples was prepared on 0.17-mm-thick glass substrates. It was shown that vacuum vapor-phase film deposition methods make it possible to control structural changes during deposition, enabling the fabrication of films with predictable optical properties. In particular, an improvement in the structural characteristics of CdTe films was observed, namely a reduction in the number of defects and in surface roughness for thicknesses of 500–2500 nm.

The use of the OPTIFIT environment enabled parametric fitting of the model parameters to the experimental data, which ultimately made it possible to obtain the optical characteristics of the thin films and to compare them with the measurement results.

It is shown that CdTe films with thicknesses of 1500–2000 nm exhibit strong absorption for wavelengths shorter than the CdTe bandgap (fundamental absorption edge) and high optical transmittance in the near-IR beyond the band-edge, which makes them promising for high-efficiency photovoltaic energy converters.

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Оптичні та структурні властивості тонких плівок CdTe для фотоелектричних застосувань

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У роботі представлено результати дослідження тонких плівок телуриду кадмію вирощених на скляних підкладках методом відкритого випаровування у вакуумі. На основі експериментально виміряних спектрів оптичного пропускання плівок розраховано їх оптичні параметри в програмному середовищі OPTIFIT. Порівняльний аналіз товщин виміряний за допомогою профілометра та модель OPTIFIT показали незначні відхилення товщини для тонких плівок з товщиною до 3-4 мкм. Аналіз АСМ зображень показав значне покращення структурних характеристик плівок CdTe, зокрема, зменшення кількості дефектів і шорсткості поверхні для товщин 500-2500 нм, що сприяє підвищенню коефіцієнта корисної дії фотоелектричних перетворювачів енергії.

Ключові слова: відновлювана енергія, тонкі плівки, CdTe, сонячні елементи, оптичні властивості, програмне забезпечення, OPTIFIT, комп'ютерне моделювання, напівпровідники.