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BOUBAKER POLYNOMIALS EXPANSION SCHEME (BPES)–RELATED OPTICAL PROPERTIES OF β-SnS_2 SPRAYED LAYERS

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β-SnS_2 layers have been prepared on glass substrates by spray pyrolysis technique at temperature $T_s \approx 270^\circ$C. The transmission-reflectance spectra, subjected to an original BPES-related protocol, led to accurate calculations of the effective absorptivity. The knowledge of lastly obtained values of the thermal diffusivity allowed the determination of the opto-thermal expansivity ψ_{AB} as a guide to evaluating the conjoint optical and thermal performances of the as-grown layers.

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1. Introduction

β-SnS_2 tin disulfide is a layered two-dimensional semiconductor with an indirect band gap at 2.2 eV. Its layered structure, as well as its gap, makes it useful for several applications. Tin disulfide and derived ternary alloys magnetic and electrical properties [1 − 4] make their compounds suitable as absorbers or window layers in photovoltaic (PV) solar cells.

In 2002, Soliman et al. [5] studied the structural and electrical properties of similar chalcogenides thin films and yielded interesting spectral response of thermal measurements. These results were confirmed by the works of B. A. Mansour et al. [6] who investigated quaternary thin layers grown at various temperatures. They carried out an interesting study of the optical behavior changes observed in the structural phases with the growth temperature during the film formation. In 2004, Salem et al. [7] prepared annealed ternary thin films on appropriate substrates and studied their interesting optical properties. More recently, El-Nahass et al. [8] reported UV spectra of metal-free phtalocyanine SnS_2-like thin films.

In most of these studies [3 − 8], the fabrication processes (deposition in acidic

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bath, electro-deposition, successive ionic layer adsorption and reaction (SILAR) etc.) were criticized to be expensive and slow. In this paper, as grown β-SnS_2 layers prepared with low-cost and rapid techniques were subjected to structural and optical investigations as guides to the determination of intrinsic characteristics.

2. Growth of layers and characterization techniques

Tin disulfide layers have been deposited on 0.5 mm thick glass substrates. The precursor solution was a mixture of $SnCl_4$ and $SC(NH_2)_2$. Precursor solution and gas flow rates were respectively 1.5 l/min and 4 l/min. Cross micrographs enabled to estimate the as-grown layers thickness. Under the mentioned conditions, the thickness of the deposited layers lie between 1.3 and 1.8 μm.

Layers transmittance and the reflectance measurements were carried out by a 400 – 2000 nm wavelength-range spectrophotometer (Shimadsu UV 3100F). XRD measurements have been carried out with a double-beam Philips (PW 3710) apparatus. Common techniques: atomic force microscopy (AFM) and scanning electron microscopy (SEM) were applied for the analyzes of layer's surface.

For calculations purposes, the thermal diffusivity of the layers has been deduced from precedent studies [9 – 10].

3. Results and discussion

3.1. Structure investigations

XRD patterns (Fig. 1) show that the layers crystallize with a strong (001) X-ray diffraction peak which indicates a strongly c-axis oriented crystallites perpendicular to the lower plane. The second minor peak (101) is also characteristic to β-structured sulfides. The surface morphology, revealed by Figs. 2a and 2b), shows a

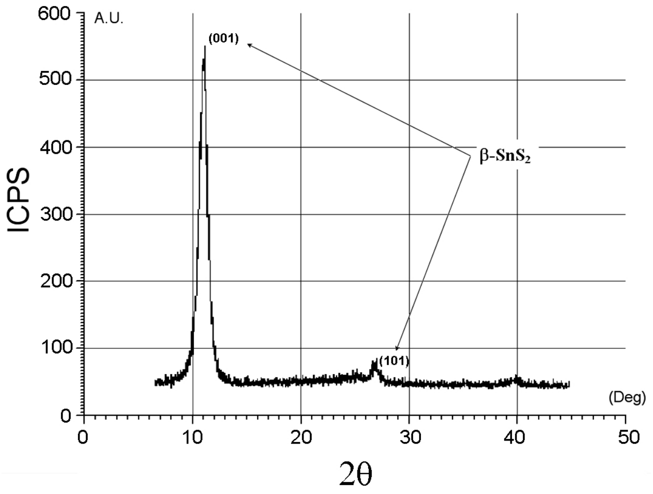

Fig. 1. X-ray diffraction spectrum of β-SnS_2 *layers.*

dense columnar structure and a periodically homogenous surface. This result is in good agreement with XRD observations.

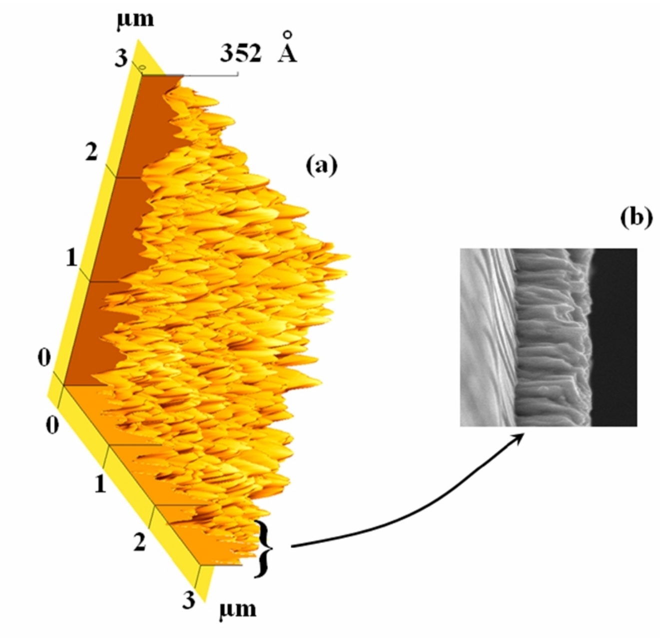

Fig. 2. (a) AFM and (b) SEM micrographs of β-SnS_2 *layers.*

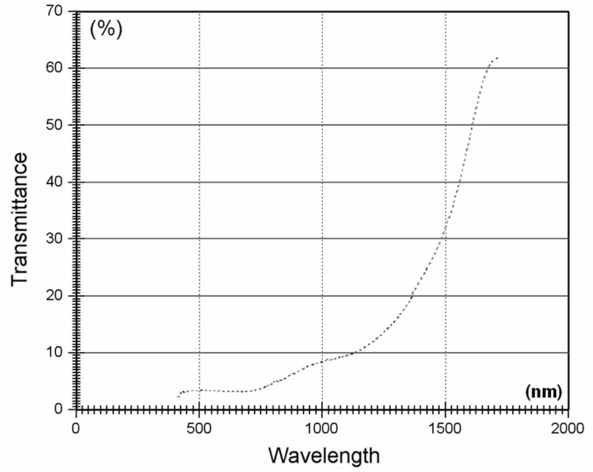

Fig. 3. Transmittance spectrum of β-SnS_2 *layers.*

3.2. Optical properties

Figures 3 and 4 present, respectively, the transmission and reflectance spectra of the as grown β-SnS_2 layers. It is noted that the transmission coefficient increases with the wavelength. The β-SnS_2 layer obtained at the temperature $T_s \approx 270°C$ is transparent both in the visible domain ($T = 40\%$) and the near-IR ($T = 70\%$). The reflectance seems to oscillate in a narrow range (20 − 25%) in the visible domain and the near-IR.

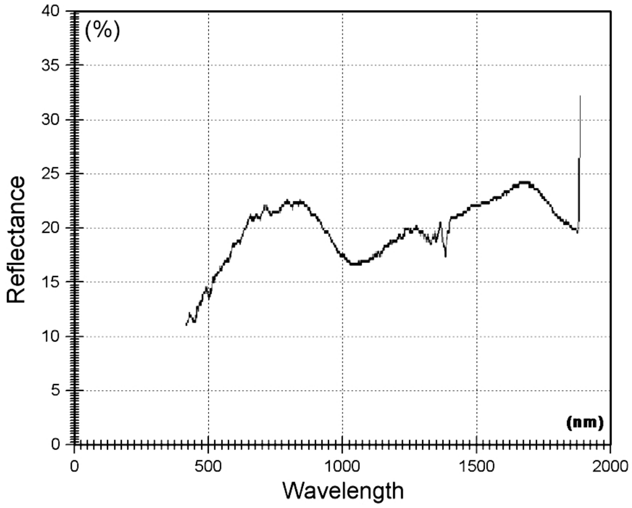

Fig. 4. Reflectance spectrum of β-SnS_2 *layers.*

The effective absorptivity $\widehat{\alpha}$ has been defined [11] as the mean normalized absorbance (Fig. 5) weighted by $I(\widetilde{\lambda})_{\mathrm{AMI\,5}}$, the solar standard irradiance, where $\widetilde{\lambda}$ the normalised wavelength

$$\widetilde{\lambda} = \frac{\lambda - \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}}\,, \quad \lambda_{\min} = 400.00 \text{ nm}\,, \quad \lambda_{\max} = 2000.00 \text{ nm}\,, \tag{1}$$

and

$$\widehat{\alpha} = \frac{\int_0^1 I(\widetilde{\lambda})_{\mathrm{AMI\,5}}\ \alpha(\widetilde{\lambda})\ \mathrm{d}\widetilde{\lambda}}{\int_0^1 I(\widetilde{\lambda})_{\mathrm{AMI\,5}}\ \mathrm{d}\widetilde{\lambda}}\,, \tag{2}$$

where $I(\widehat{\lambda})_{\mathrm{AMI\,5}}$ is the Reference Solar Spectral Irradiance, fitted using the Boubaker polynomials expansion scheme (BPES) [12 − 17]

$$I(\widetilde{\lambda})_{\mathrm{AMI\,5}} = \frac{1}{2N_0} \sum_{1}^{N_0} \theta_n B_{4n}(\widetilde{\lambda}\,\beta_n)\,,$$

where β_n are the Boubaker polynomials [14 − 17], B_{4n} the minimal positive roots, θ_n the given coefficients, N_0 is a given integer, and $\alpha(\widetilde{\lambda})$ is the normalized absorbance spectrum. In precedent studies [9 − 11], the normalized absorbance spectrum was deduced from the BPES, applied to the set of m experimental measured values of the transmittance-reflectance vector $\left(T_i(\widetilde{\lambda}_i);\, R_i(\widetilde{\lambda}_i)\right)\Big|_{i=1,\cdots m}$ versus the normalized wavelength $\lambda_i\Big|_{i=1,\cdots m}$ defined in Eq. (1)

$$R(\widetilde{\lambda}) = \frac{1}{2N_0}\sum_{n=1}^{N_0} \xi_n \; B_{4n}(\widetilde{\lambda}\,\beta_n) \tag{3}$$

$$T(\widetilde{\lambda}) = \frac{1}{2N_0}\sum_{n=1}^{N_0} \xi_n' \; B_{4n}(\widetilde{\lambda}\,\beta_n) \tag{4}$$

where β_n are the minimal positive roots of 4n-Boubaker polynomials B_{4n} [13 − 16], N_0 is a prefixed integer and ξ and ξ' are coefficients which minimize the square sums

$$\bar{\omega} = \sum_{i=1}^{n}\left[\left(R_i(\lambda_i) - \frac{1}{2N_0}\sum_{q=1}^{N_0}\xi_q\, B_{4q}(\lambda_i\,\beta_q)\right)^2 + \left(T_i(\lambda_i) - \lim_{N_0\to\infty}\frac{1}{2N_0}\sum_{q=1}^{N_0}\xi_q'\, B_{4q}(\lambda_i\,\beta_q)\right)^2\right] \tag{5}$$

Finally, the normalized absorbance spectrum is calculated using the relation

$$\alpha(\widetilde{\lambda}) = \frac{1}{d}\sqrt[3]{\left|\ln\left(\frac{0.08}{1-T(\widetilde{\lambda})}\right)\ln\left(\frac{1}{(1-T(\widetilde{\lambda})}\right)\ln\left(\frac{0.64}{1-T(\widetilde{\lambda})}\right)\right|} \quad \text{for } \lambda\in[400;\ 1000]\,\text{nm}\,, \tag{6}$$

$$\alpha(\widetilde{\lambda}) = \frac{1}{d}\sqrt[3]{\left|\ln\left(\frac{0.3}{1-T(\widetilde{\lambda})}\right)\ln\left(\frac{1}{(1-T(\widetilde{\lambda})}\right)\ln\left(\frac{0.09}{1-T(\widetilde{\lambda})}\right)\right|} \quad \text{for } \lambda\in[1000;\ 2000]\,\text{nm},$$

where d is the layer thickness.

Equations (6) can be simplified as

$$\alpha(\widetilde{\lambda}) = \frac{2.311}{d}T(\widetilde{\lambda}) = \frac{2.311}{d}\left(1 - \frac{1}{2N_0}\sum_{n=1}^{N_0}(\xi_n + \xi_n')\, B_{4n}(\widetilde{\lambda}\,\beta_n)\right) \quad \text{for } \widetilde{\lambda}\in[0.0;\ 0.25]\,\text{a.u.}, \tag{7}$$

$$\alpha(\widetilde{\lambda}) = \frac{2.047}{d}T(\widetilde{\lambda}) = \frac{2.047}{d}\left(1 - \frac{1}{2N_0}\sum_{n=1}^{N_0}(\xi_n + \xi_n')\, B_{4n}(\widetilde{\lambda}\,\beta_n)\right) \quad \text{for } \widetilde{\lambda}\in[0.25;\ 1.0]\,\text{a.u.}$$

The profile $\alpha(\widetilde{\lambda})$ of the room-temperature grown layer is presented in (Fig. 5). The effective absorptivity $\widehat{\alpha}$ is calculated using Eqs. (2) and (7).

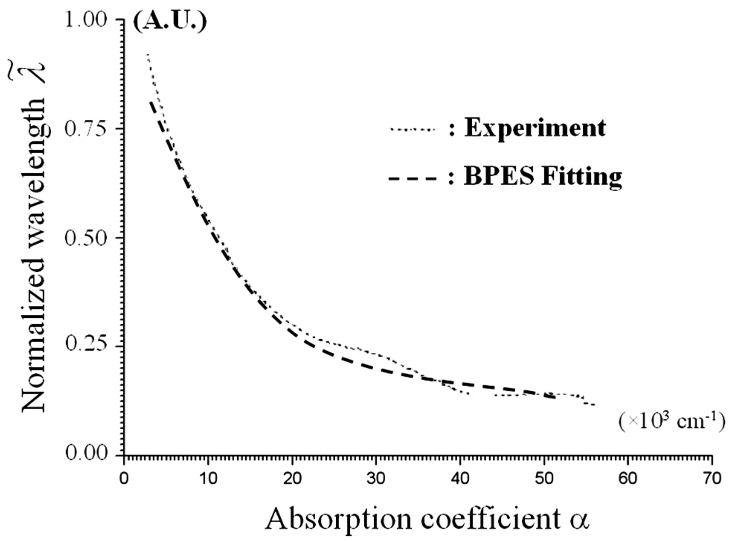

Fig. 5. Absorption coefficient α versus wavelength λ of β-SnS_2.

3.3. Determination of Amlouk-Boubaker opto-thermal expansivity ψ_{AB}

The Amlouk-Boubaker opto-thermal expansivity ψ_{AB} is defined [11] by

$$\psi_{AB} = \frac{D}{\widehat{\alpha}} \tag{8}$$

where D is the thermal diffusivity of layer's material and $\widehat{\alpha}$ is defined in Eq. (2). The value of this parameter, which is expressed in m^3/s, is assimilated to a 3D expansion velocity of the transmitted heat inside the material.

The calculated values of the mean normalized absorbance $\widehat{\alpha}$ and the Amlouk-Boubaker opto-thermal expansivity ψ_{AB} , are shown in Table 1.

TABLE 1. Values of the Amlouk-Boubaker opto-thermal expansivity ψ_{AB}.

Parameter	Value	Unit
D	14.5×10^{-6}	m^2s^{-1}
$\widehat{\alpha}$	25.5×10^{3}	cm^{-1}
ψ_{AB}	5.68×10^{-12}	m^3s^{-1}

The obtained value, $\psi_{AB} = 5.68 \times 10^{-12} m^3s^{-1}$, of the Amlouk-Boubaker opto-thermal expansivity allows comparison with the performance of already investigated binary sulphide-like compounds [11, 18, 19].

4. *Conclusion*

In this paper, spray pyrolysis deposited β-SnS_2 layers have been investigated. Conjoint XRD, AFM and SEM observations indicate a columnar structure and a periodically homogenous surface. Optical measurements based on the reflectance and transmittance allowed evaluating some relevant optothermal parameters like the mean normalized absorbance $\widehat{\alpha}$ and the Amlouk-Boubaker opto-thermal expansivity ψ_{AB}. The relatively low value of the latter parameter is a very promising result since it implies that this material heat retaining capability is lower than of similar compounds [18, 20 − 23].

Our future investigations are oriented toward deepening Boubaker polynomials expansion scheme (BPES) applications [24 − 33] as well as obtaining detailed thermal response of the layered β-SnS_2 structures when subjected to modulated heat-light excitations.

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BOUBAKEROVA SHEMA RAZVOJA PO POLINOMIMA (BPES) I OPTIČKA SVOJSTVA PRSKANIH SLOJEVA β-SnS_2

Na staklenoj podlozi priredili smo slojeve β-SnS_2 metodom vrućeg prskanja na temperaturi 270°C. Spektri prolazne i odrazne svjetlosti, izvedeni primjenom nove sheme razvoja po Boubakerovim polinomima, omogućili su točno određivanje efektivne apsorptivnosti. Konačno dobiveni podaci za termalnu difuzivnost omogućili su određivanje opto-termičkog širenja ψ_{AB} kao vodilju za određivanje povezanih optičkih i termičkih svojstava svježe pripremljenih slojeva.