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Effect of substrate temperature on the optical and structural properties of CdS nano particles

Wpływ temperatury podłoża na właściwości optyczne i strukturalne nanocząstek CdS

Thin films of CdS have been deposited on glass substrates using the chemical spray pyrolysis method at different substrate temperatures of 100°C, 150°C, 200°C, and 250°C to investigate the optimum temperature to prepare CdS particles with nano dimensions. The CdS thin film was examined using SEM, X-ray spectrum analysis, and UV--visible spectrophotometry. The SEM images and X-ray spectra were used to estimate the structural features and grain size of the films. The optical properties and optical constants also varied clearly with temperature. In addition, the energy gap changed with temperature from 2.1 eV to 2.55 eV.

Keywords: CdS thin films, optical properties of CdS, chemical spray pyrolysis, CdS nanoparticles

Cienkie warstwy CdS zostały osadzone na szklanych podłożach metodą chemicznej pirolizy natryskowej w temperaturach podłoża wynoszących 100°C, 150°C, 200°C i 250°C w celu określenia optymalnej temperatury do przygotowania cząstek CdS o wymiarach nano. Tak przygotowane próbki zostały zbadane za pomocą SEM i spektrofotometrii UV-VIS, przeprowadzono także analizę widma rentgenowskiego. Obrazy SEM i widma rentgenowskie zostały wykorzystane do oszacowania cech strukturalnych i wielkości ziarna warstw. Właściwości optyczne i stałe optyczne zmieniały się wyraźnie wraz ze zmianą temperatury. Przerwa energetyczna wynosiła w zależności od temperatury od 2,1 eV do 2,55 eV.

Słowa kluczowe: cienkie warstwy CdS, właściwości optyczne CdS, chemiczna piroliza natryskowa, nanocząstki CdS

1. Introduction

Cadmium sulphide (CdS) is an important II–VI group semiconductor material owing to its optical properties, photoconductivity, high electron affinity, and stability [1]. Cadmium sulphide is the most studied chalcogenide with an energy gap of 2.42 eV [2]. It exhibits *n*-type conductivity due to its native defects such as sulphur vacancies and interstitial cadmium [3], and it possesses crystal structures including cubic and hexagonal [4]. Cadmium sulphide thin film has many applications in technical fields, such as heterojunction solar cells [5], light-emitting diodes [6], field-effect transistors [7, 8], photovoltaics [9], and detectors [10]. A thin film of cadmium sulphide can be deposited using several methods, such as RF sputtering [11], chemical bath deposition [12], thermal evaporation [13], spray pyrolysis [14], and close spaced sublimation (CSS) techniques [15]. In our study, thin films of cadmium sulphide have been deposited on glass substrates at different substrate temperatures over the range of 100°C, 150°C, 200°C, and 250°C; the films were then examined using several modern techniques such as scanning electron microscopy (SEM), X-ray spectrum analysis, and UV-visible spectrophotometry.

2. Experimental

Cadmium sulphide thin films have been deposited on glass substrates by chemical spray pyrolysis. The substrates were cleaned ultrasonically using methanol, acetone, and distilled water,

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Table 1. Deposition parameters of the chemical spray pyrolysis technique
Tabela 1. Parametry osadzania w technice chemicznej pirolizy natryskowej

Specification	Deposition parameters
Chemical compounds [g]	$CdCl_2$: 0.3
	Na_2S: 0.4
Deposition temp. [°C]	100
	150
	200
	250
Number of sprays	20
Spray rate [ml/min]	5.7
Pressure [kg/cm^2]	7.5
Distance [cm]	25

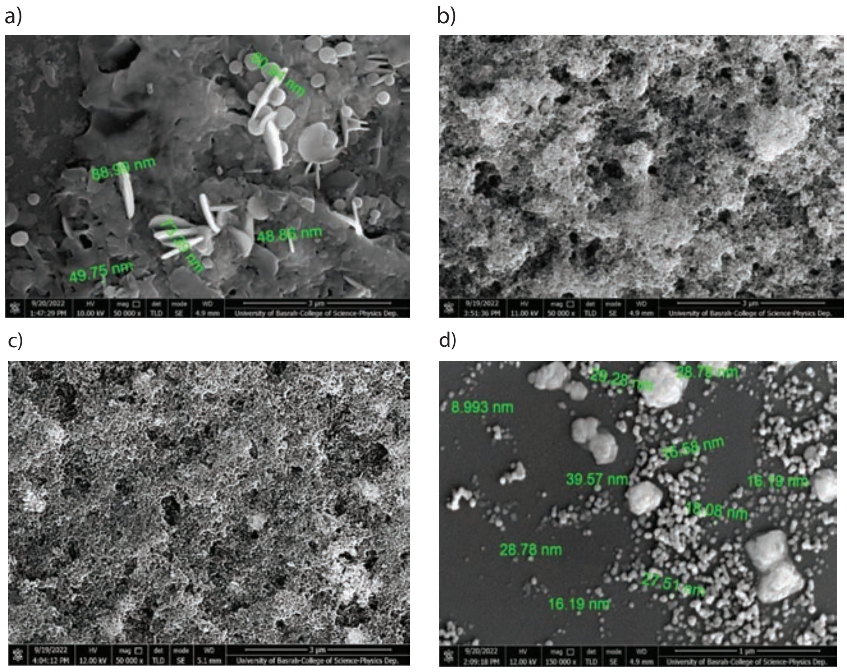

Fig. 1. Scanning electron microscope images of CdS thin films prepared at different temperatures: a) 100°C, b) 150°C, c) 200°C, d) 250°C

Rys. 1. Obrazy SEM cienkich warstw CdS przygotowanych w różnych temperaturach: a) 100°C, b) 150°C, c) 200°C, d) 250°C

Table 2. Grain diameter variation with deposition temperature based on SEM images
Tabela 2. Zmiana średnicy ziarna w zależności od temperatury osadzania na podstawie obrazów SEM

Substrate temperature [°C]	Grain diameter [nm]
100	68
150	36
200	30
250	23

Table 3. Grain size variation with deposition temperature based on X-ray spectrum
Tabela 3. Zmiana wielkości ziarna w zależności od temperatury osadzania na podstawie widma rentgenowskiego

Temperature [°C]	Grain size [nm]
100	54.08
150	32.4
200	27.19
250	17.97

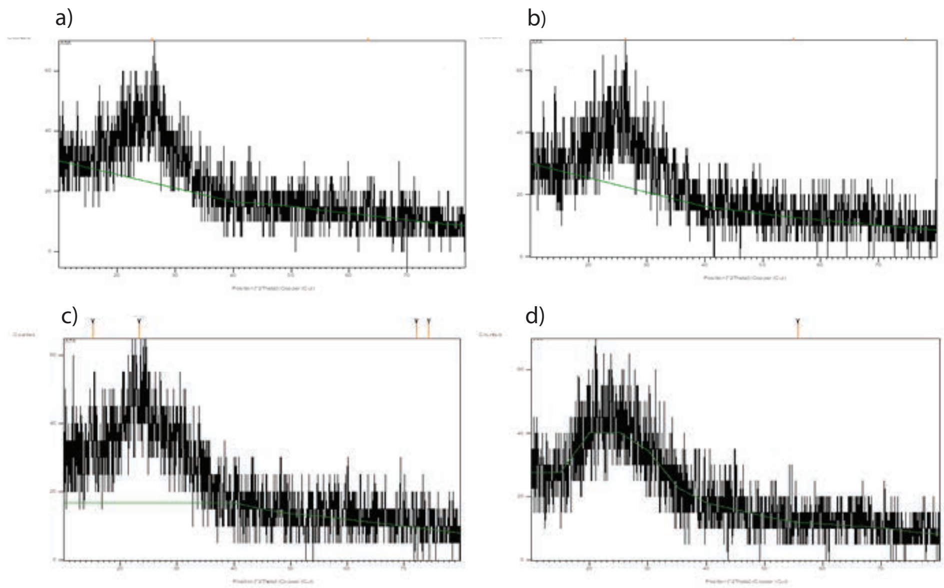

Fig. 2. X-ray spectra of CdS thin films prepared at different temperatures: a) 100°C, b) 150°C, c) 200°C, d) 250°C

Rys. 2. Widmo rentgenowskie cienkich warstw CdS przygotowanych w różnych temperaturach: a) 100°C, b) 150°C, c) 200°C, d) 250°C

after which the slides were left to dry in a clean room. Cadmium Cd^{+2} was obtained by dissolving 0.3 g of cadmium chloride ($CdCl_2$) in 50 ml of distilled water, while sodium sulphide was produced by dissolving 0.4 g of sodium sulphide in 50 ml of distilled water. Both solutions were then mixed in a 100 ml beaker and the mixture was stirred for 1 hour on a magnetic stirrer at 80°C. The substrate temperatures during the deposition process varied and assumed values of 100°C, 150°C, 200°C, and 250°C, while the other parameters were maintained constant as shown in table 1.

Table 4. Energy gap variation with deposition temperature
Tabela 4. Zmiana wartości przerwy energetycznej w zależności od temperatury osadzania

Temperature [°C]	Energy gap [eV]
100	2.55
150	2.55
200	2.3
250	2.1

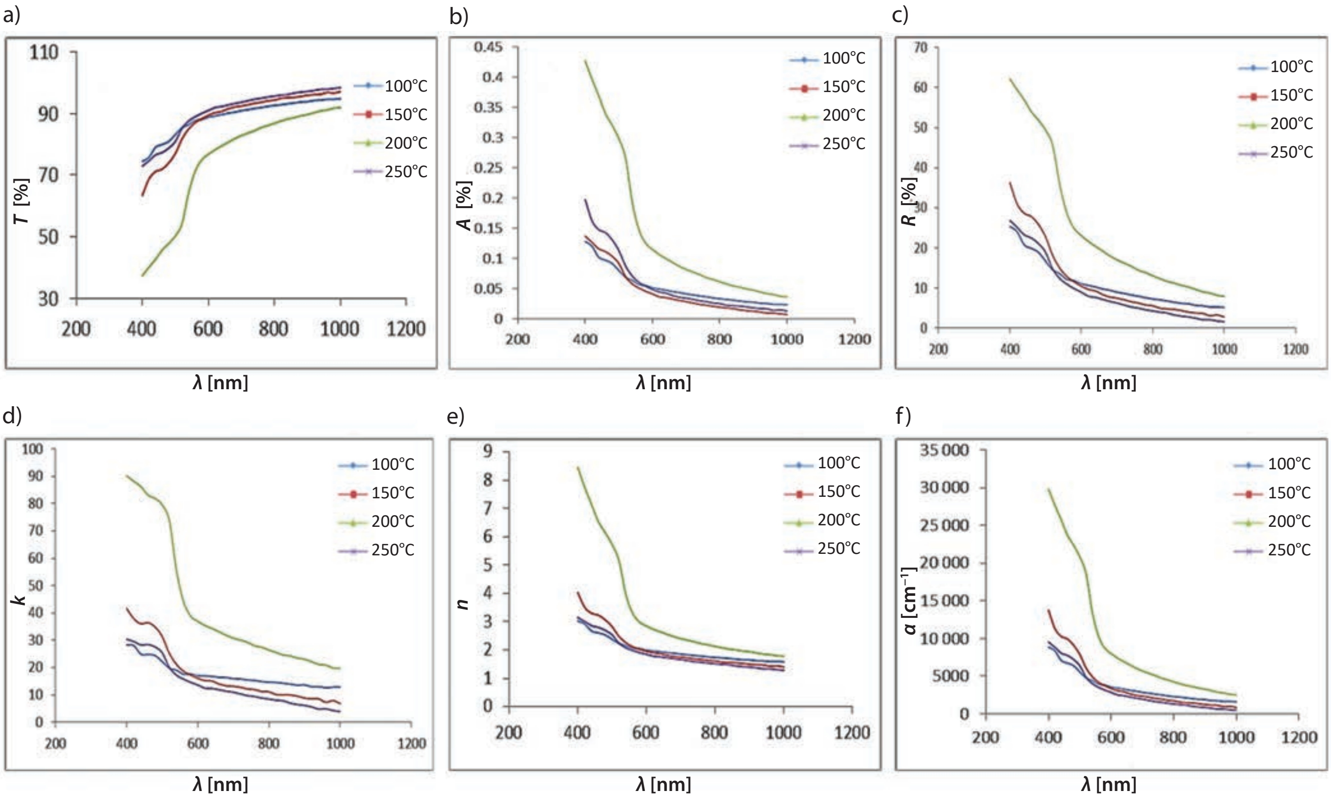

Fig. 3. Optical properties at the wavelength of CdS thin films prepared at different temperatures: a) transmittance, b) absorbance, c) reflectance, d) extinction coefficient, e) refractive index, f) absorption coefficient

Rys. 3. Właściwości optyczne i długość fal cienkich warstw CdS przygotowanych w różnych temperaturach: a) transmitancja, b) absorbancja, c) współczynnik odbicia, d) współczynnik ekstynkcji, e) współczynnik załamania światła, f) współczynnik absorpcji

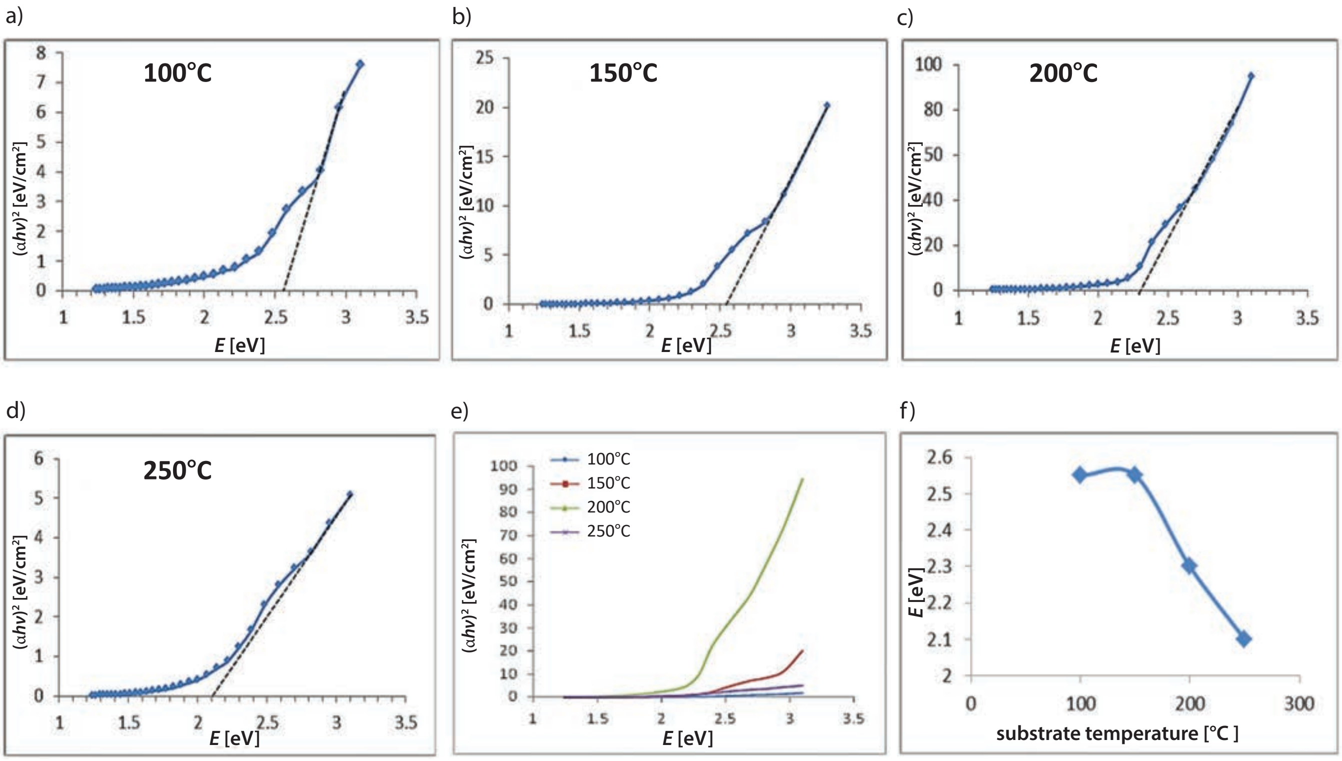

Fig. 4. The effect of substrate temperature on the energy gap: a) energy gap for film prepared at 100°C, b) energy gap for film prepared at 150°C, c) energy gap for film prepared at 200°C, d) energy gap for film prepared at 250°C, e) energy gap for films prepared in various temperatures, f) energy gap value according to temperature

Rys. 4. Wpływ temperatury podłoża na przerwę energetyczną: a) przerwa energetyczna dla warstwy przygotowanej w temperaturze 100°C, b) przerwa energetyczna dla warstwy przygotowanej w temperaturze 150°C, c) przerwa energetyczna dla warstwy przygotowanej w temperaturze 200°C, d) przerwa energetyczna dla warstwy przygotowanej w temperaturze 250°C, e) przerwy energetyczne dla warstw przygotowanych w różnych temperaturach, f) wartość przerwy energetycznej w zależności od temperatury

3. Results and discussion

Scanning electron microscope images indicate that the grain size decreases with temperature (Fig. 1). The average size of the grains varied from 54 nm for the films prepared at 100°C, to 17 nm for the films prepared at 250°C which agrees with the X-ray spectrum as shown in Tables 2, 3. The decrease in grain size occurs as a result of the drying of the solution drops before they reach the hot substrates, which negatively affects their adhesion to the substrates and prevents the growth and aggregation of the grains.

The X-ray spectra show that all the films are amorphous with a slight presence of the crystalline phase (Fig. 2). It is worth mentioning that the crystalline phase increases with temperature during the deposition and this agrees with the SEM images (Fig. 1). The grain size was calculated from the X-ray spectrum using the Scherrer equation.

The transmittance, absorbance, reflectance, extinction coefficient and refractive index were measured for the films. The transmittance decreases at 100°, 150° and 200°C, but there is crossing at 550 nm. A negative effect was shown at 250°C as a result of the decreasing film thicknesses caused by high temperatures preventing the growth and aggregation of films thus indicating that the film was converted to nano-grain medium. However, after 600 nm the effect of temperature is approximately constant. Accordingly, an inverse effect happens with absorbance and reflectance, which varied over the wavelength range from 400 nm to 550 nm, which afterwards remain constant for the higher wavelengths (Fig. 3).

The energy gaps have been calculated for cadmium sulphide thin films prepared at different temperatures. The energy gap was 2.55 eV for both films prepared at temperatures of 100°C and 150°C, 2.3 eV for films prepared at 200°C, and 2.1 eV for the film prepared at 250°C as shown in table 4. The variation in the optical properties and optical constants may result from the variation in the film structures and grain size (Fig. 4).

4. Conclusions

Scanning electron microscope images and X-ray spectra show that the grain size decreased with substrate temperature and the films were amorphous with a slight presence of a crystalline phase. The energy gaps have been calculated for cadmium sulphide thin films prepared at different temperatures, where the energy gap was 2.55 eV for both films prepared at 100°C and 150°C, 2.3 eV for films prepared at 200°C, and 2.1 eV for the film prepared at 250°C.

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