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RESEARCH ARTICLE - MATHEMATICS

Investigate the influence of Al content on the structure and surface morphology of Al:CdS-PVA nanocomposites

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Abstract

In this study, Al:CdS-PVA nanocomposites thin films were prepared on glass substrates by the chemical bath deposition (CBD) method. The impact of aluminum (Al) concentrations of (0, 0.04, 0.08, and 0.12) M on the crystal structure and morphology characteristics of the prepared nanocomposites film was investigated. XRD tests show that all of the samples have a polycrystalline crystal structure with a cubic phase for CdS. The (111) plane is the preferred orientation. The Al:CdS-PVA film crystallinity improved, and the crystallite size increased with the increase in Al concentrations. The surface morphology from FESEM images showed that the Al:CdS-PVA nanocomposites film surface is porous. The AFM results showed that surface roughness and RMS values increased with an increasing of impurity.

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Keywords: Cadmium sulfide, polyvinyl alcohol, aluminum, nanocomposites, thin film.

1. Introduction

Nanocomposites consisting of organic polymers and nanoparticles are considered a form of material that has sparked tremendous interest. [1]. Nanocomposites are useful for sensors, solar cells, and optoelectronic, etc [2-5]. Thin film technology is crucial to solid-state physics due to its wide applications in diverse fields of industry. Where it was developed many new areas of technology by thin film technology [6].

Cadmium sulfide (CdS) are one of the semiconductors of the n-type with acceptable transparency and a wide direct band gap of 2.42eV [7, 8] Polymer matrices provide good controllability, so the use of polymers in thin film fabrication has attracted great attention [9]. Polyvinyl alcohol (PVA) was first prepared by Hermann and Haehnel in 1924. PVA is a granular powder that is translucent, odorless, tasteless, and white-colored. It is soluble in water [10,11]. PVA has advantages such as a large energy gap [12] and is an organic candidate for hosting nanoparticles to generate thin films. [13,14], There are various methods used to deposit CdS films, like those created by chemical bath deposition (CBD) [15]. Various researchers have intensively explored CdS-PVA nanocomposites because of the broad CdS band gap and the good, elastic mechanical characteristics of PVA [16].(Saikia et al. 2011) By combining silver nitrate and cadmium acetate, Ag is doped into a CdS-PVA thin film. in a 103:1 Ag:CdS ion ratio. The films were nanocrystalline, homogeneous, and appropriate for solar cell use. Silver doping in a the solar cell's conversion capacity went to 5.63% thanks to thin film. [17]. (Nathera. 2013)have reported that CdS/PVA films were synthesized by spray pyrolysis, the films were deposited at different thicknesses. The PVA improved the crystalline quality, the films have good physical properties, and the direct band gap value of the CdS/PVA films is (2.425-2.75) eV, and are well suited for solar cell applications.[18]. (Jumi et al. 2013)have published about the synthesis of polyvinyl alcohol and cadmium sulfide: copper nanoparticles (PVA/CdS:Cu).The sizes of (NCs) obtained by TEM are very close to those obtained by XRD. Photoluminescence (PL) from the band edge emission (481 nm) is shown. The obtained results indicate the possible applications of the LED-shaped fabricated samples and nanodevices [19]. (Vishwakarma et al. 2014) This study discusses the investigation of the structural and optical characteristic, of CdS (NPs) that were synthesized in the PVA matrix. XRD patterns showed the hexagonal phase of nanoparticles. The calculated grain size is found to be 3.62 nm, and the obtained results can be useful in the fabrication of photonic devices [20]. (Vaneeta et al. 2015) Pure and doped CdS/PVA nanocomposites (Al, Ga, and

In) have been studied. DC conductance (σd). They were measured at temperatures varying between 288 to 333 K. The results showed that the change in current is symmetrical and linear with voltage at temperatures (less than 300 K), and the addition of III elements to the CdS-PVA thin films leads to a reduction in the optical conductivity[21]. (Hussein et al. 2018) reported the use of the (CBD) technique to create pure and aluminum doped CdS films. With increases in aluminum concentration, the crystallite size rises. The AFM results showed an increase in roughness and the RMS value. It was also discovered that doping increased the absorption coefficient, the calculations showed the optical energy gap values for pure CdS thin films and doped with different percentages (0, 2.5, 5, and 7.5%) were (2.89, 2.85, 2.79, and 2.81) volts, respectively [22]. (Abdel-Galil et al. 2020) successfully fabricated CdS/PVA nanocomposites. The size of CdS nanoparticles is less than 20 nm, and the size of the CdS grain changes with irradiation doses. improved the PVA electrical conduction through γ-irradiation and adding CdS, which can be used in optoelectronic devices [23]. In the work, the structure, and morphology characteristics of Al:CdS-PVA deposited by (CBD), were studied at various concentrations of aluminum.

2. Experimental Setups

Chemical bath deposition was used to prepare the Al:CdS-PVA samples. First, we dissolve 2g of polyvinyl alcohol (PVA) powder in 100 mL of deionized water with a magnetic stirrer at 70 °C and add a concentration of 0.1 M of cadmium sulfate ($CdSO_4$) to a PVA solution at 70 °C with a continuous stirrer. After that, the solution is left to cool completely to obtain complete and good cadmium sulfate solubility. NH_4OH is added to adjust the pH of the solution to about 11. About 24 hours later, thiourea [$CS(NH_2)_2$] was dissolved at a concentration of 0.1 M in deionized water (100 mL). The solution of thiourea was mixed with the base material solution with continuous stirring at room temperature until it began to gradually turn a light yellow color. substrates were inserted into the solution vertically and kept for 24 hours at room temperature. Then it is taken out and thoroughly washed. A suitable amount of aluminum nitrate ($Al(NO_3)_3.9H_2O$) solution is added to the matrix solution before the addition of thiourea. Table 1 shows the ratios of the aluminum and PVA-$CdSO_4$ solution.

Table 1: ratios of aluminum and PVA-CdSO4 solution.

Ratios	Al (mL)	PVA-$CdSO_4$ (mL)
0 %	0	100
4 %	4	96
8 %	8	92
12 %	12	88

3. Result and Discussion

3.1. Crystalline Structure

X-ray diffractometer (multi-purpose DX-2700BH) Was used to examine the samples of Al:CdS-PVA, which were fabricated by the CBD technique, to reach the X-ray diffraction results (XRD). From table 1, the results of the examination showed that the films have a cubic phase and polycrystalline structure; there is more than one peak at diffraction angles 2θ of 26.4°, 31.5°, 43.8°, and 51.9°, which are plane-indexed. (111), (200), (220), and (311). The preferred growth trend for all concentrations appeared at the (111) diffraction plane for angles 2θ of (26.519, 26.391, 26.368, and 26.467), respectively. There are no diffraction peaks prominently associated with aluminum doping, indicating that Al atoms are successfully solved in the CdS structure [3, 14], as shown in Figure 1. The results are completely identical to the standard card (JCPDS No. 75-0581) and results [18, 24, 25]. Adding aluminum affected the crystal growth in the prepared films, which is highly consistent with [26]. Bragg's law, $2d\sin\theta = n\lambda$, allows us to calculate the values of the spacing (d) between the planes (hkl), while calculating the value of the lattice constant

(a) by Eq. (1) [15]. The results obtained, shown in Table 2, are in good agreement with the values in JCPDS No. 75-0581 and the [15, 27].

$$a_{cubic} = d_{hkl}\,(h^2 + k^2 + l^2)^{1/2} \quad (1)$$

From Figure 1, it can be noticed that the peaks intensity increases with increasing concentrations of aluminum doping, which indicates a rise in crystallinity. The crystallite size, D, was estimated from the Scherer's eq. [2,28]:

$$D = \frac{K\lambda}{\beta\, COS\, \theta} \quad (2)$$

Where (K ≈ 0.94), (λ ≈ 1.5405 Å), and β is the full width at half the maximum intensity (FWHM) of the peaks.

Table 2: X-ray parameters of Al:CdS-PVA nanostructure film in various concentrations of Al orientation along the (111) plane.

Structural Parameters	0 Al	0.04 Al	0.08 Al	0.12 Al
2θ(deg)	26.467	26.368	26.391	26.519
$d_{observed}$ (Å)	3.364	3.377	3.374	3.358
d_{JCPDS}(Å)	3.366	3.366	3.366	3.366
FWHM(deg)	0.809	0.538	0.463	0.604
Lattice Constants a。 (Å)	5.827	5.849	5.843	5.816
Crystalline Size (D) nm	9.833	14.909	17.332	13.205
$N_o \times 10^{17}\ m^{-2}$	13. 144	3. 771	2.400	5.427
$\delta \times 10^{15}\ m^{-2}$	10.340	4.498	3.328	5.734
Strain $\times 10^{-3}$	3.524	2.324	1.999	2.624

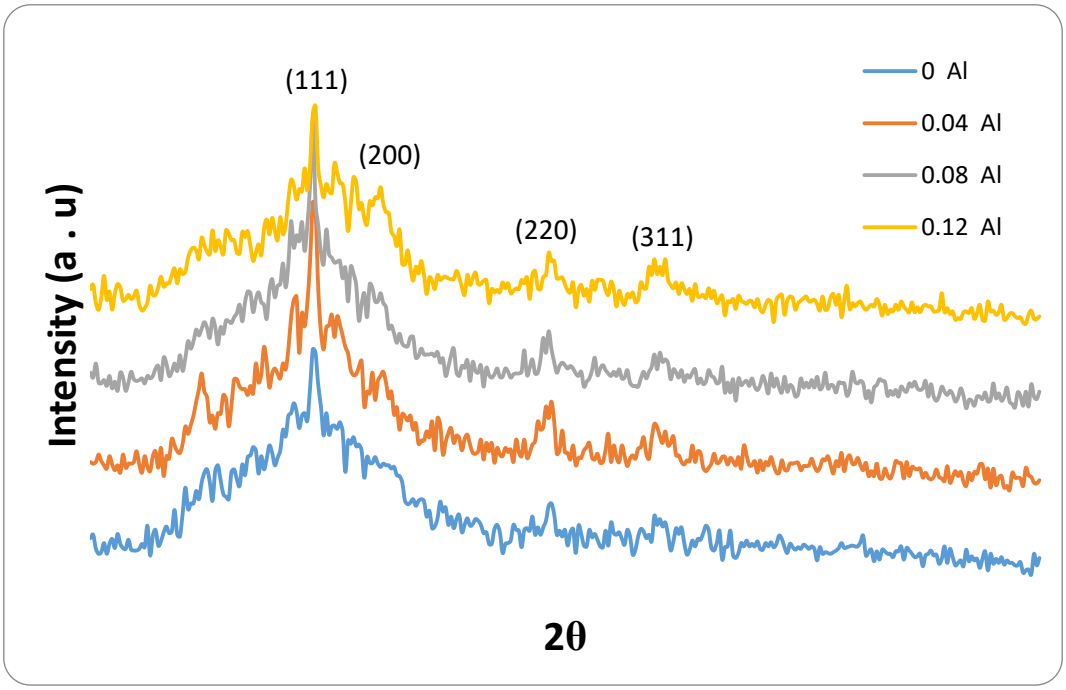


Figure 1: The XRD of Al:CdS-PVA nanostructure film prepared at Al concentrations.

The crystallite size values for the films are shown in Table 2. It is noted that the size of the crystals in the case of doping with Al has increased compared to the pure state. An increase in crystallite size can indicate an improvement in the crystallization state of the film and a decrease in crystalline defects[14, 29]. From Table 2, the intensity of dislocations reduces with the an increase in the particle size and the average strain value decreases as the particle size increases. The results agree with S. Rajathi et al. [30], and the value of the dislocation density (δ) and the value of the mean strain (ε) can be calculated using Eq (3) and (4) [31].

$$\delta = \frac{1}{D^2} \tag{3}$$

$$\varepsilon = \frac{\beta cos\theta}{4} \tag{4}$$

3. 2. Surface morphology

Surface morphology was investigated of Al:CdS-PVA films by field emission scanning electron microscopy (FESEM). Surface nature of the film deposited at various Al concentrations (0, 0.04, 0.08, and 0.12) M is shown in figure 2. The inset images reveal to the FESEM images at higher magnifications and at the 500nm scale of the samples. The FESEM micrograph showed the homogeneity of the surface and grain uniform distribution over the substrate, which has a porous web structure. Doping with Al did not change the structure. This can be explained by the fact that the Al^{3+}, which has a radius of 0.45 Å, is smaller than the radius of Cd^{2+}, which is equal to 1.03 Å. The results are consistent with [22, 32, 33].

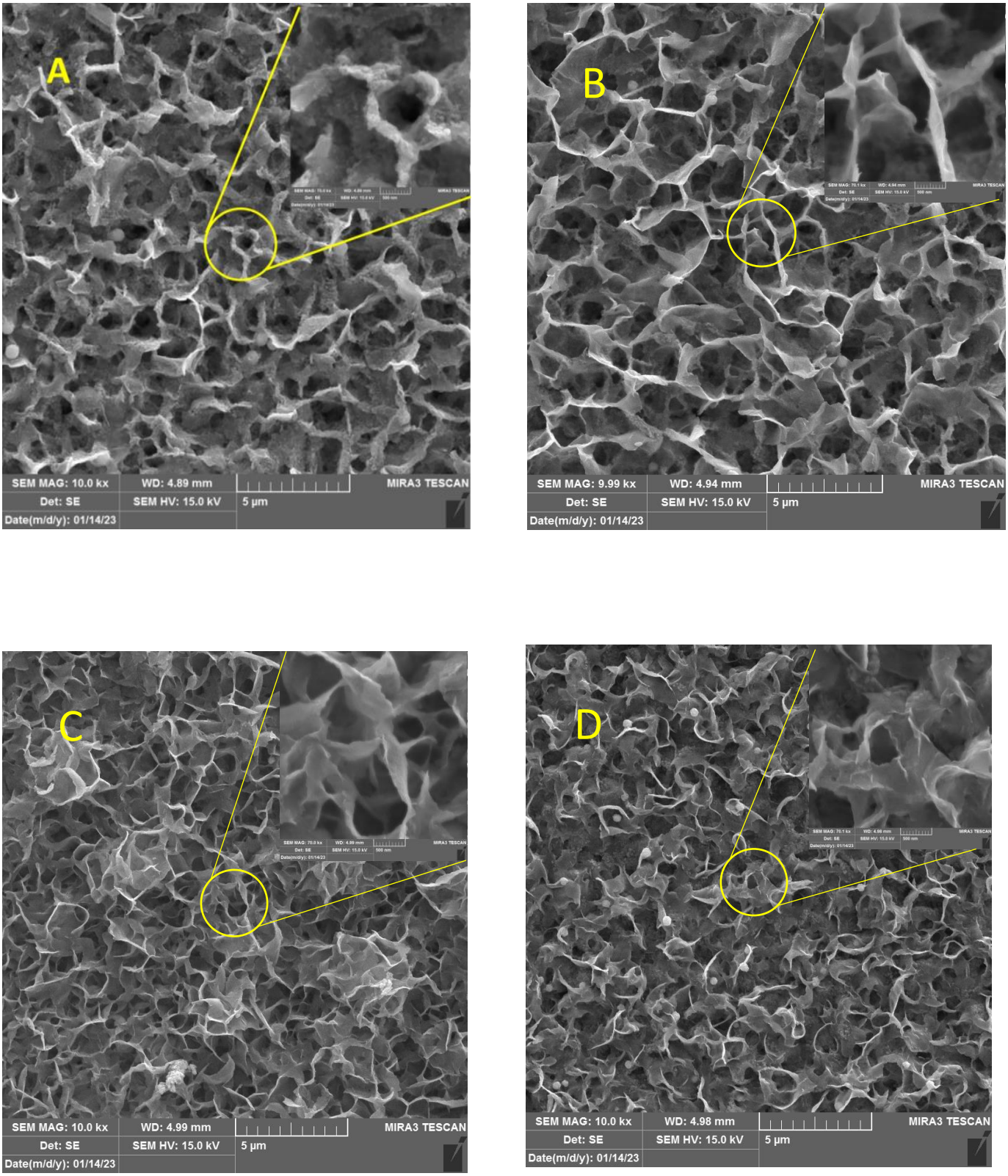


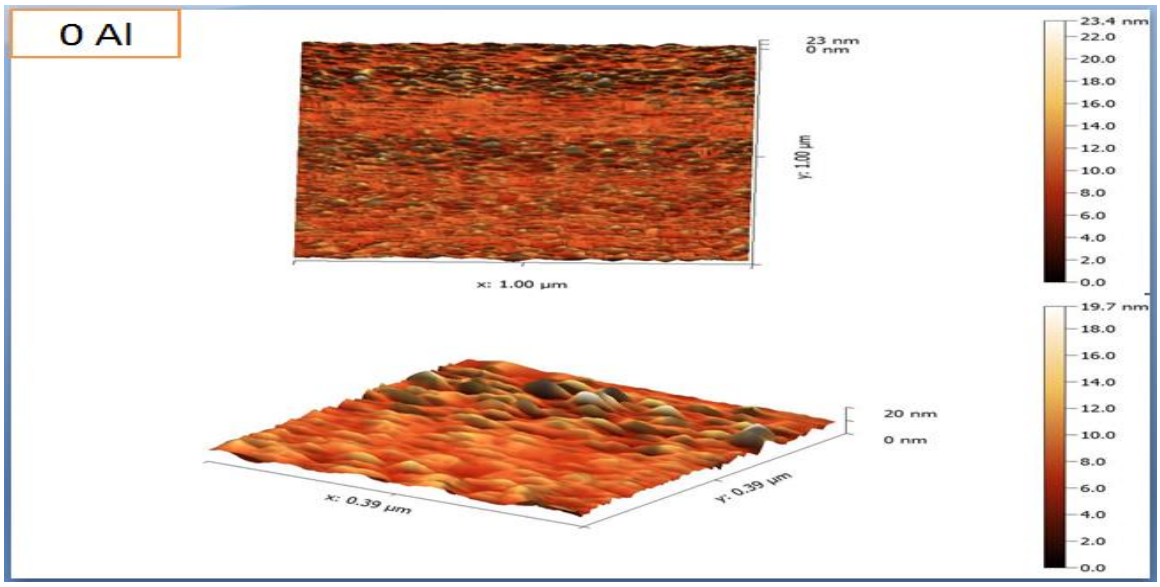
Figure 2: FESEM of Al:CdS-PVA at Al concentrations (0, 0.04, 0.08, and 0.12) M.

3. 4. Atomic force microscopy (AFM)

AFM has the ability to analyze surfaces and give accurate information about their topographical properties [34]. The AFM two- and three-dimensional images of Al-doped CdS-PVA nanocomposites prepared at different aluminum concentrations (0, 0.04, 0.08, and 0.12) are presented in figure 4. From the images. The film surface has homogeneity, good grain distribution, and is pinhole-free due to improved crystallization of the film state. Table 3 shows the average roughness (Ra) and root mean square roughness (RMS). The surface roughness and RMS values vary with the increasing percentage of impurity; they increase when the percentage increases from 0.04 to 0.08, then decrease when it reaches 0.12. This reflects the accuracy of the tests, where these results correspond to those obtained from FESEM analysis and XRD. The results are consistent with the literature [17, 22].

Table 3: AFM data of Al:CdS-PVA nanocomposites at Al concentrations.

AFM Parameters	0 Al	0.04 Al	0.08 Al	0.12 Al
RMS (nm)	1.67	1.68	2.08	1.48
Ra (nm)	1.21	1.27	1.52	1.06



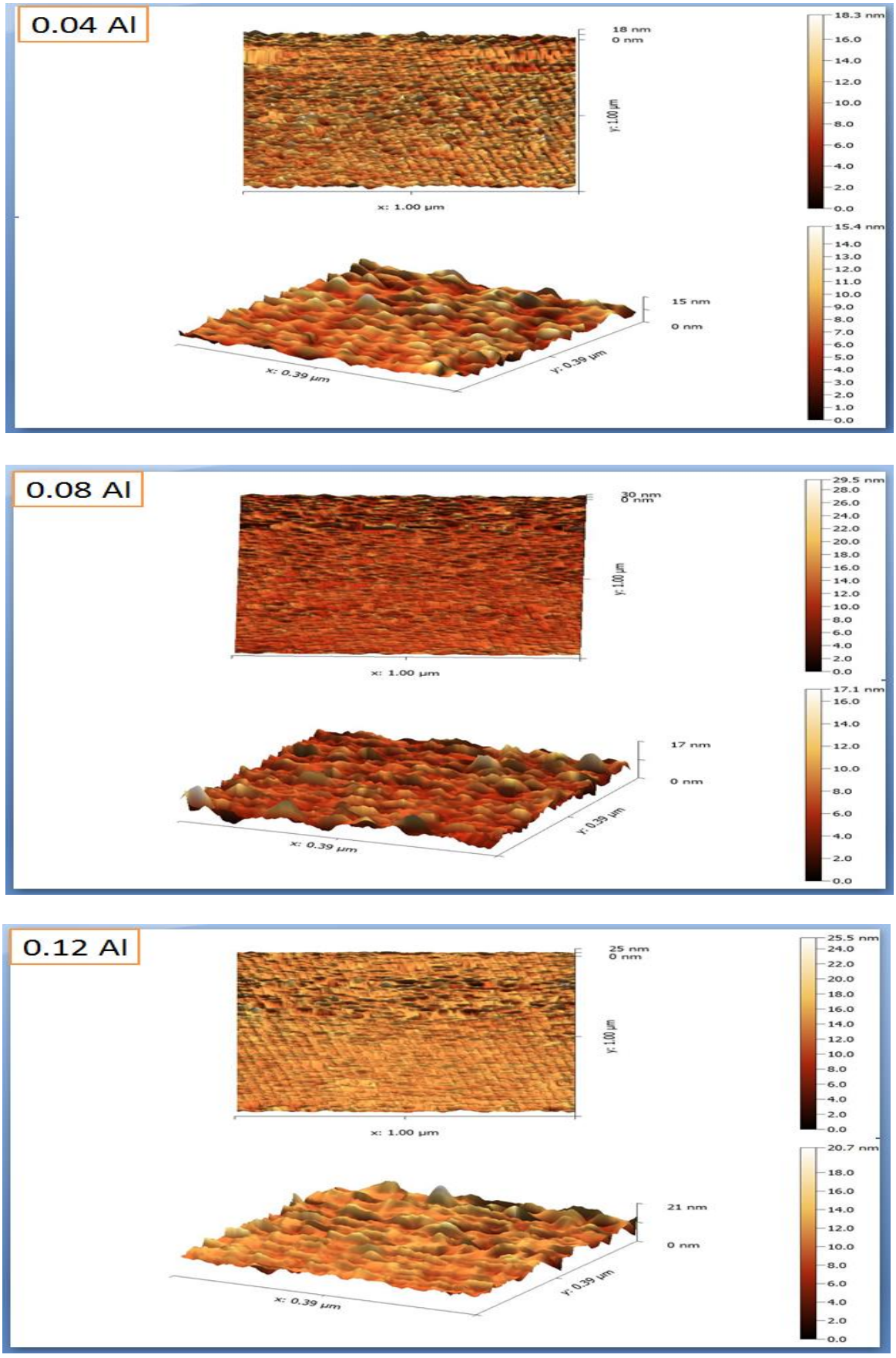


Figure 3: AFM images of Al:CdS-PVA at Al concentrations (0, 0.04, 0.08, and 0.12) M.

4. Conclusion

The CBD method was used to deposit Al:CdS-PVA nanocomposites at Al concentrations (0, 0.04, 0.08, and 0.12 M). Increasing the concentration has an effect on the structural and morphological characteristics of the nanocomposites. The XRD analysis revealed a polycrystalline cubic phase structure and an increasing crystallite size with increasing Al. The FESEM micrograph showed the homogeneity of the film's surface and its porous structure. The AFM results showed that as Al concentrations increased from 0 to 0.08, there was an increase in the values of each film's roughness and root mean square (RMS), then it decreased at a concentration of 0.12.

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