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A Study of the Structural, Optical, Properties of Au/CdS Films Prepared by Laser Pulsed Deposition Method

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دراسة الخصائص التركيبية والبصرية لأغشية الذهب/كبريتات الكادميوم بطريقة الترسيب النبضي بالليزر

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ABSTRACT

Background:

Numerous studies have confirmed the importance of manufacturing solar cells and photodetectors as well as different types of sensors. This is due to their essential rolls in many industries.

Working methods:

Two materials, gold (metal) and cadmium sulfate were used, which waspowder pressed at 15 megapascals pressure in a disc form with a 2 cm diameter.(PLD) technique was used to form thin films, where the number of pulses was changed and the laser power was fixed at 100 millijoules with a 1064 nanometers wavelength.

Results:

Au/CdS film exhibited a polycrystalline structure with a hexagonal lattice, The presence of gold in the CdS material resulted in very low lattice strain, as the atomic radii of CdS (0.154 nm) and Au (0.165 nm) are closely matched

Conclusions:

This study revealed The possibility of manufacturing cadmium sulfate films with Au by thermal diffusion method. The current and voltage values of the prepared solar cell increase with the increase of the layers of thin films on the surface of the solar cell, thus increasing the lighting current, as direct energy transfer occurs. X-ray examinations of the films prepared by the pulsed laser deposition method showed that they have a polycrystalline structure and a hexagonal lattice. The films prepared in the case of CdS-Au showed the size of the grains of the thin films increases with the increase of the laser energy and the number of pulses. We also note that the surface roughness decreases with the decrease of the concentration.

Keywords: Deposition; nanoparticles, solar cells, visible spectroscopy, gas sensors

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INTRODUCTION

Nanomaterials are characterized by their small size ranging from 1 to 100 nm, and possess unique properties that make them widely used in various applications [1, 2]. Nowadays, Lasers, with their narrow bandwidth and high power density, have become essential tools for material processing, including the production of thin films using techniques such as pulsed laser deposition (PLD) [1, 2]. PLD includes focusing a pulsed laser beam onto the surface of a target solid material, resulting in rapid evaporation and the formation of highly excited and ionized species that are deposited on a substrate [3]. To achieve optimal film properties, the use of inert gases such as argon is more common [5].

In this study, we focus on two materials: gold and cadmium sulfide. Gold, a solid and highly conductive metal, has excellent chemical resistance making it to be used in various applications [7, 8]. Cadmium sulfide, an inorganic material, is commonly used as a substitute for impurities and serves as a primary source of cadmium [10, 11]. Laser technology plays a crucial role in the fabrication and processing of these materials, as its powerful light beam can evaporate even the most heat-resistant materials [11].

To investigate the synthesis of thin films, a PLD setup is used, where the target and substrate are placed in a high-level vacuum chamber connected to vacuum pumps [11]. This research aims to explore the properties and applications of gold-cadmium sulfide films fabricated using laser ablation, contributing to the advancement of nanomaterials fabrication and their potential applications as solar cells.

Materials and Methods

The pure gold material, with a purity rate of (99.99), was purchased from accredited gold dealers, while the (CDS) material was purchased from one of the chemical offices approved to import such materials, and after conducting complete tests to ensure the validity of the material, it was used in the work.

- **Methods**

Figure 1 shows a schematic diagram of a simple PLD system. The laser beam inlet and other auxiliary ports can bring oxidation-preventing purge gas and additional attachments into the system. Outside the chamber, a lens with a known focal length is used to focus the laser beam on the target surface from which the thin films are made [12,13].

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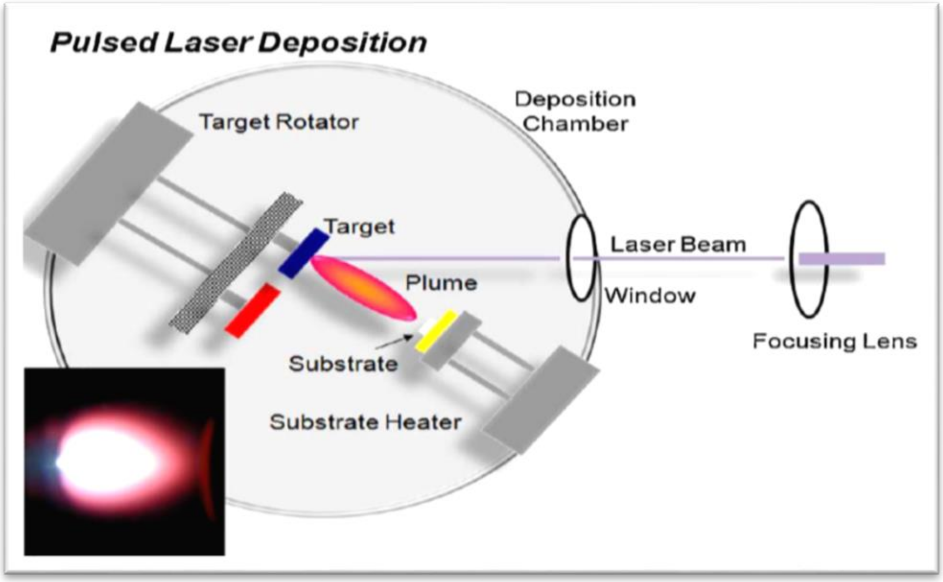

Figure 1. shows a picture illustrating the pulsed laser deposition system [14]

RESULTS AND DISCUSSION

X-ray diffraction (XRD) analysis was performed to investigate the crystal structure and orientation of the films. The XRD patterns in Figures (2, 3) revealed that both the CdS film and the Au/CdS film exhibited a polycrystalline structure with a hexagonal lattice, characteristic of CdS. The CdS film showed prominent peaks at angles of (25.13°, 26.74°), and 28.24° corresponding to the (100), (002), and (101) planes, respectively. Similarly, the Au/CdS film exhibited peaks at angles of (25.13°, 26.66°), and 28.20° for the same planes. These XRD patterns matched the standard data card of CdS (ICDD card no. 41-1049). The XRD analysis also indicated a preferred orientation along the (002) plane.

The crystallite sizes of the films, calculated using Scherrer's formula, were found to be within the nanoscale range. The presence of gold in the CdS material resulted in very low lattice strain, as the atomic radii of CdS (0.154 nm) and Au (0.165 nm) are closely matched. This absence of strain suggests a high crystallization with low density of dislocations and minimal lattice distortion in the film structure. The lattice parameters (a and c) of the films were also calculated using equations (3.4) and found to be in close agreement with the standard data card of CdS (a= 4.1 Å, c= 6.7 Å) and Table 1 The data of XRD measurements of the films.

$$\delta = \frac{1}{D^2} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (2)$$

$$a = \sqrt{1/3}\,\lambda/\sin\theta \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (3)$$

$$c = \lambda/\sin\theta \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (4)$$

$$\varepsilon = \beta\cos\theta/4 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (5)$$

$$TC\,(hkl) = \frac{I(hkl)/I_o(hkl)}{N^{-1}\ \sum_N I(hkl)/I_o(hkl)} \qquad (6)$$

where N is the number of diffraction peaks, I (hkl), I_o (hkl) are the measured and the standard intensity

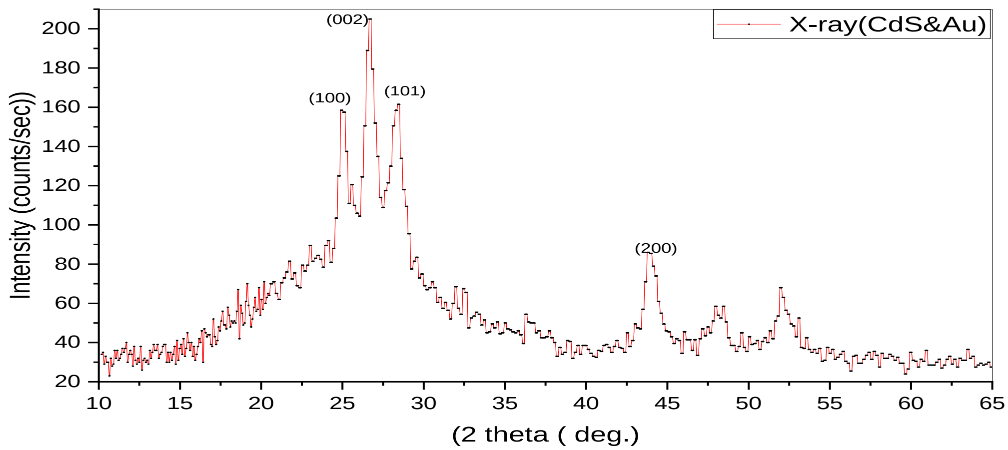

Figure 2: Shows the X-ray diagram of CdS & Au elements [17]

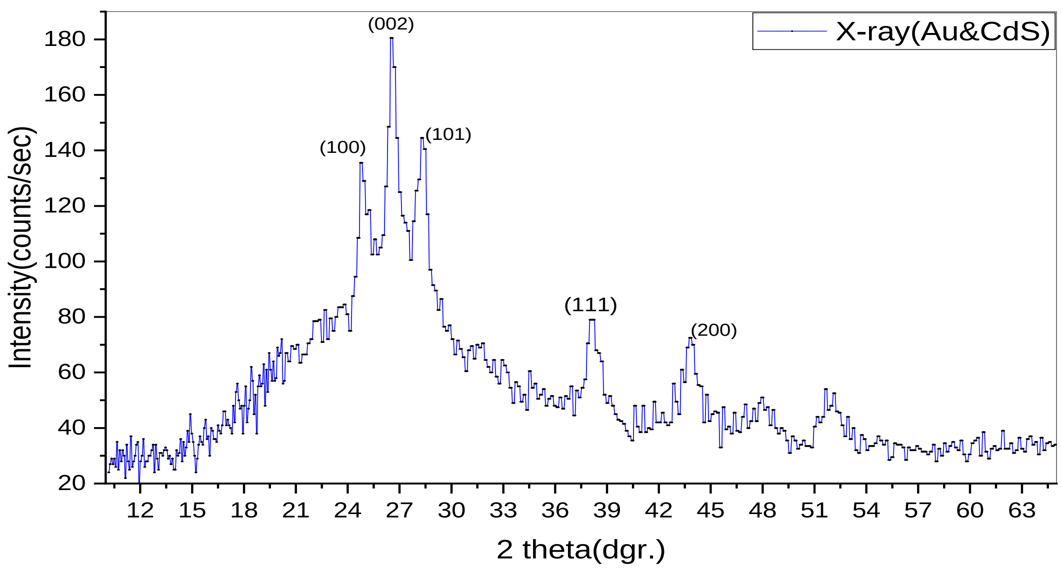

Figure 3: Shows the X-ray diagram of Au & CdS elements[15]

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Table 1. The data of XRD measurements of the films

Samples	2θ (deg)	d (A˚)	B(deg)	(hkl)	D (nm)
CdS	*25.130*	*3.540*	*1.280*	*(100)*	*6.36*
	26.741	3.331	1.253	(002)	6.51
	28.245	*3.156*	*1.626*	*(101)*	*5.04*
Au/CdS	25.130	3.540	1.760	(100)	4.62
	26.661	*3.340*	*1.493*	*(002)*	*5.47*
	28.205	3.161	1.520	(101)	5.39

Table 2. Structural parameters of preferred plane (002) of the films

Samples	δ×10-2 (1/nm2)	a (Å)	c (Å)	ε	TC
CdS	*2.35*	*3.84*	*6.66*	*0.00531*	*1.102*
Au/CdS	3.34	3.86	6.69	0.00633	1.011

- **AFM (Atomic Force Microscopy)**

AFM (Atomic Force Microscopy) measurements were conducted to analyze the surface characteristics of the thin film. The AFM images (Figures 5, 6, and 7) revealed that the film exhibited a relatively homogeneous distribution of atoms, forming clusters with spherical grains [16, 17]. However, the presence of different-sized spherical grains resulted in unavoidable surface roughness, as observed in the statistical tables accompanying each figure [5, 6, 7]. The formation of these clusters is attributed to the presence of two layers of nano-gold and nano-cadmium sulfate, as well as the threshold limit and differences in laser energy and the number of pulses used during the fragmentation process of the target material. These factors collectively contribute to the roughness observed on the film surface [16].

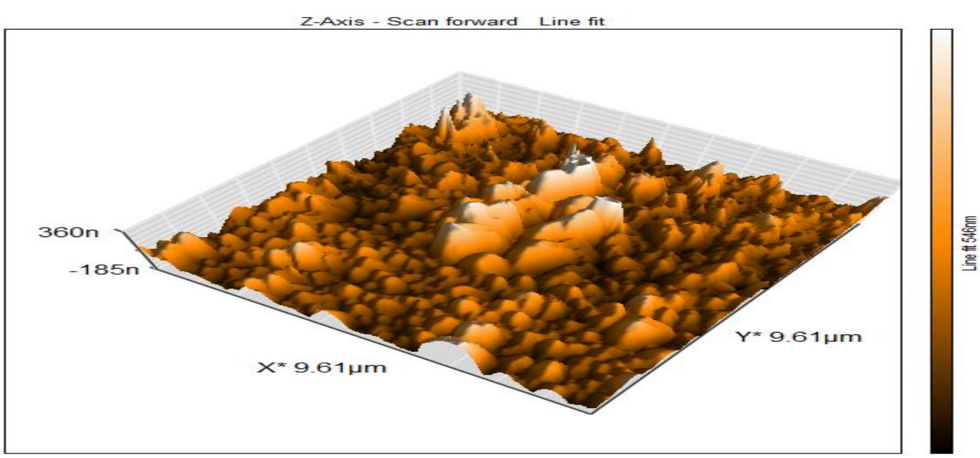

Figure 4: Shows a three-dimensional image of the surface of CdS & Au films

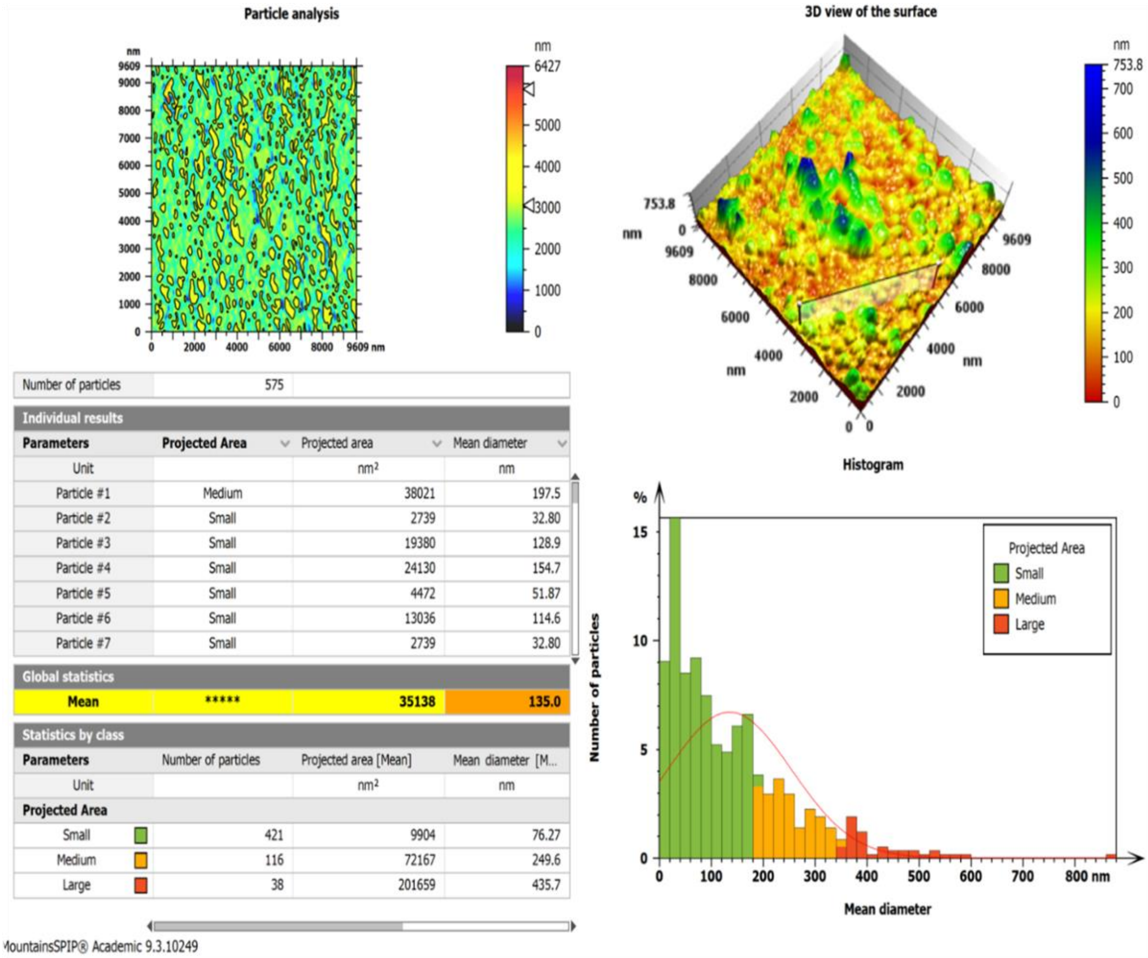

Figure 5: Shows the statistical plot of the particle size distribution of CdS & Au

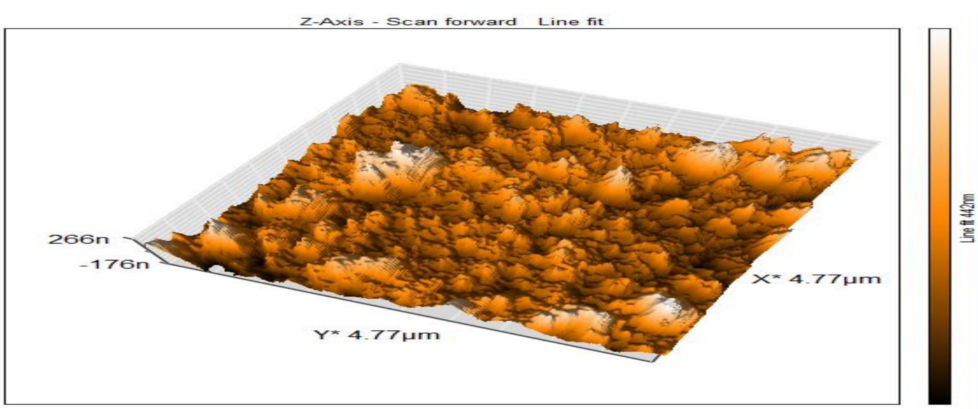

Figure 6: Shows a three-dimensional image of the surface of Au & CdS films.

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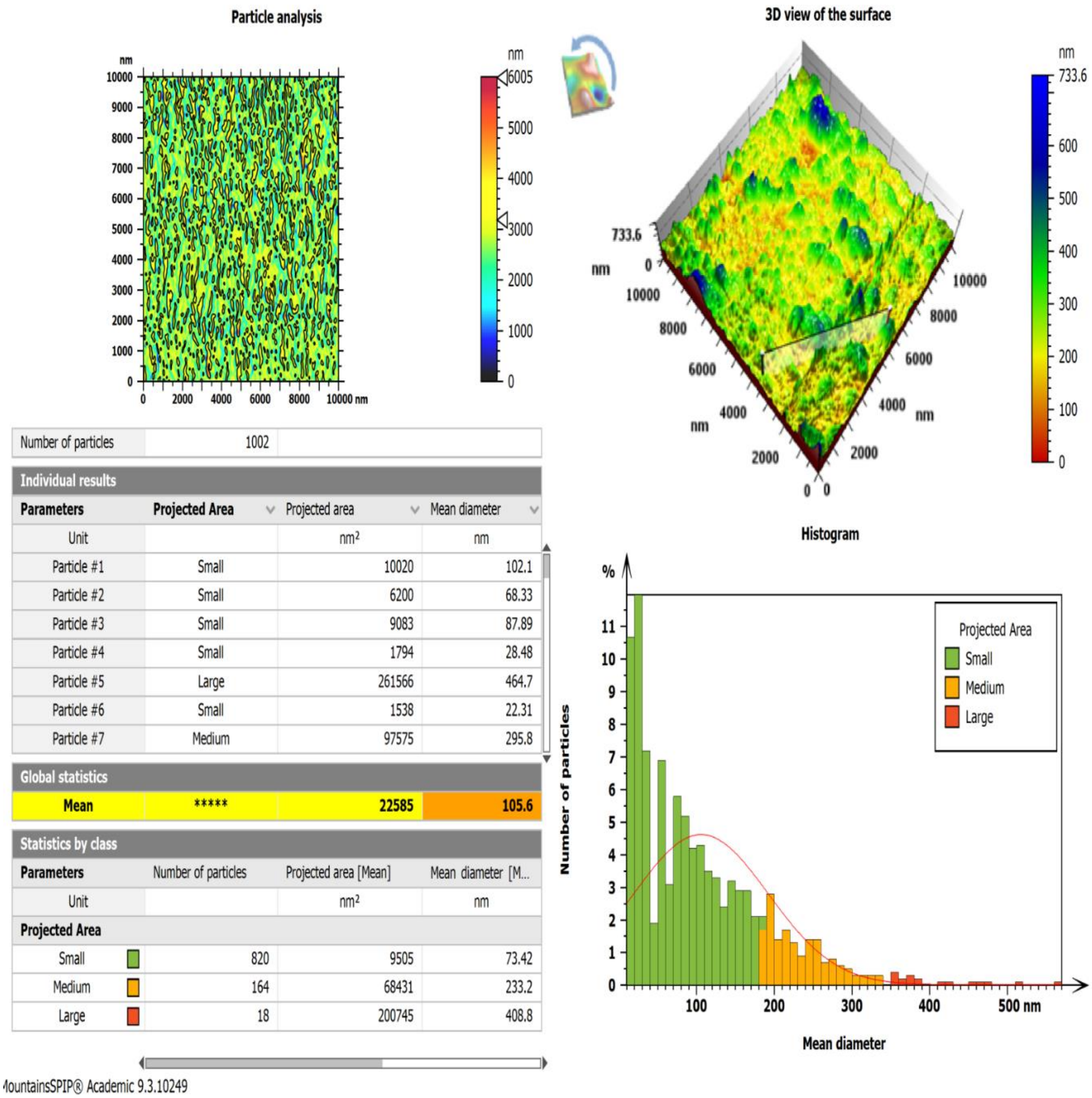

Figure 7: Shows the statistical plot of the particle size distribution of Au & CdS

- **Optical properties**
- **A- Absorption**

The ability of the prepared films to absorb light depends on the incident photon energy, material type, and crystal structure. Figure 7 displays the absorption spectra of nano-gold (Au) and cadmium sulfide (CdS) films, showing the relationship between wavelength and absorbance. As the photon energy increases (wavelength decreases), the absorbance increases gradually for both films. This increase becomes significantly steeper when the incident photon energy surpasses the optical bandgap of the materials. These observations suggest direct electronic transitions occurring within the films, with an absorption range spanning 350 nm to 550 nm. Furthermore, compared to individual materials, the mixed Au/CdS film exhibits a redshift in its peak absorption wavelength, reaching 430 nm. This shift indicates an effective interaction between Au and CdS nanoparticles, potentially tailoring the absorption properties for specific applications.

Figure 8 complements these findings by visualizing the band structure of the individual materials and the mixed composite. As shown, the conduction band of Au lies above the valence band of CdS, creating a hetero-junction at their interface. This configuration facilitates the transfer of photo excited electrons from CdS to Au, potentially enhancing the film's charge separation efficiency and contributing to improved solar cell performance.

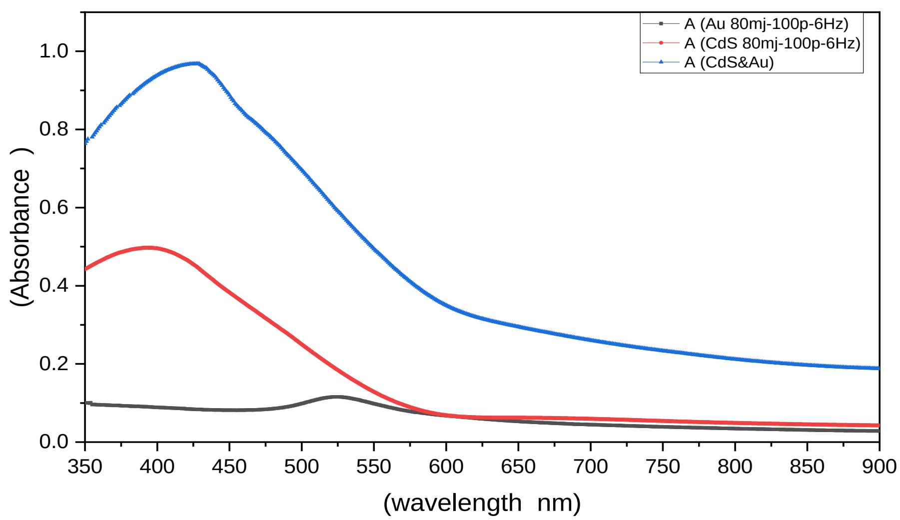

Figure 8: Shows the Absorbance spectrum of gold and cadmium sulfate.

- **Transmittance**

As expected, the transmittance of the nano-gold (Au) and cadmium sulfide (CdS) films exhibits an inverse relationship with absorbance. Figure 9 clearly shows this correlation, where peaks in absorbance, corresponding to high energy absorption, coincide with dips in transmittance, indicating low light transmission. This behavior confirms the law of energy conservation, which states that the sum of absorbed, reflected, and transmitted light must equal the total incident light. In other words, as absorption increases, the remaining transmittance must decrease to maintain this balance.

Figure 9 further elucidates this principle. We observe that when the absorbance values peak around 400 nm, the transmittance plunges to its lowest levels. This finding aligns with the direct electronic transitions observed in the absorption spectra, implying efficient light absorption within the films at these wavelengths.

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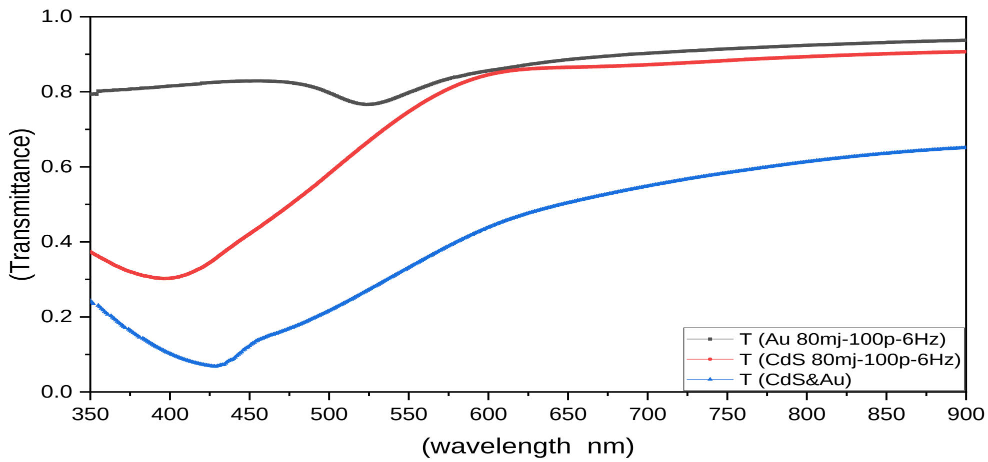

Figure 9: Shows the Transmittance spectrum of gold and cadmium sulfate.

Table 3 highlights the distinct light absorption and transmission behaviors of gold (Au), cadmium sulfide (CdS), and their combined thin film (CdS-Au) at specific wavelengths. Au exhibits peak absorption at 525 nm (green-yellow region) with moderate intensity (A=0.12) and allows most light (T=0.78) to pass through at this wavelength. In contrast, CdS demonstrates higher absorption around 399 nm (violet-blue region) with an A value of 0.5, indicating stronger light capture, but transmits only 30% (T=0.30) of light at this point.

Interestingly, combining CdS and Au creates a thin film with a significantly shifted absorption peak, reaching its maximum at 437.5 nm compared to the individual materials. This shift suggests a potential modulation of light absorption properties by combining these materials. Importantly, the CdS-Au film exhibits a very high absorption value (A=0.98) at its peak, implying efficient light capture at this wavelength. However, this is accompanied by minimal light transmission (T=0.07), hinting at its potential suitability for applications requiring efficient light absorption and conversion into other forms of energy, such as in solar cells.

- **Absorption coefficient**

The reason lies in the fact that the amount of optical absorption begins to increase when the wavelength exceeds the amount of the cut-off wavelength because the incident photons with energy greater than the value of the energy gap increase the practical value of the absorption coefficient, as it is evident from the figure that shows that all films prepared for gold and cadmium sulfate have Absorption coefficient values greater than 104 P, and this fulfills the condition that direct transfers occur if the mixing process takes place between the two materials.

As for what we noticed when preparing each membrane individually, the absorption coefficient value was less than 104, indicating that the transition here was indirect, as shown in the figure (10)

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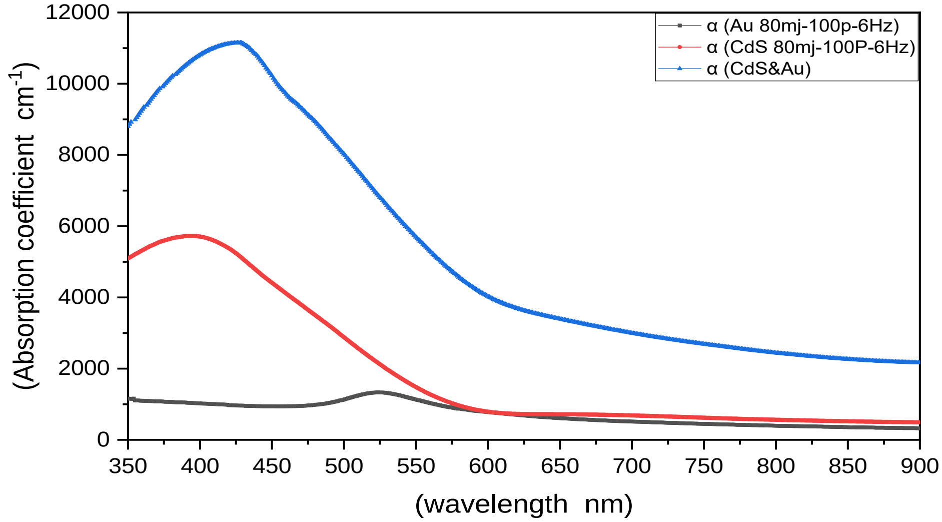

Figure 10: Shows the spectrum of the Absorption coefficient of gold and cadmium sulfate

- **Extinction coefficient**

The figure (11) shows the extinction coefficient of gold (Au) and cadmium sulfide (CdS) thin films prepared by laser pulse deposition (PLD). The extinction coefficient is a measure of how strongly light interacts with a material, encompassing both absorption and scattering. It is denoted by the symbol K in the figure (11). Higher extinction coefficient values indicate that more light is attenuated by the material. The extinction coefficient curves for Au and CdS show trends similar to absorption coefficient (α) curves, indicating that absorption is the dominant mode of light interaction in these thin films across the measured wavelength range (350-900 nm).

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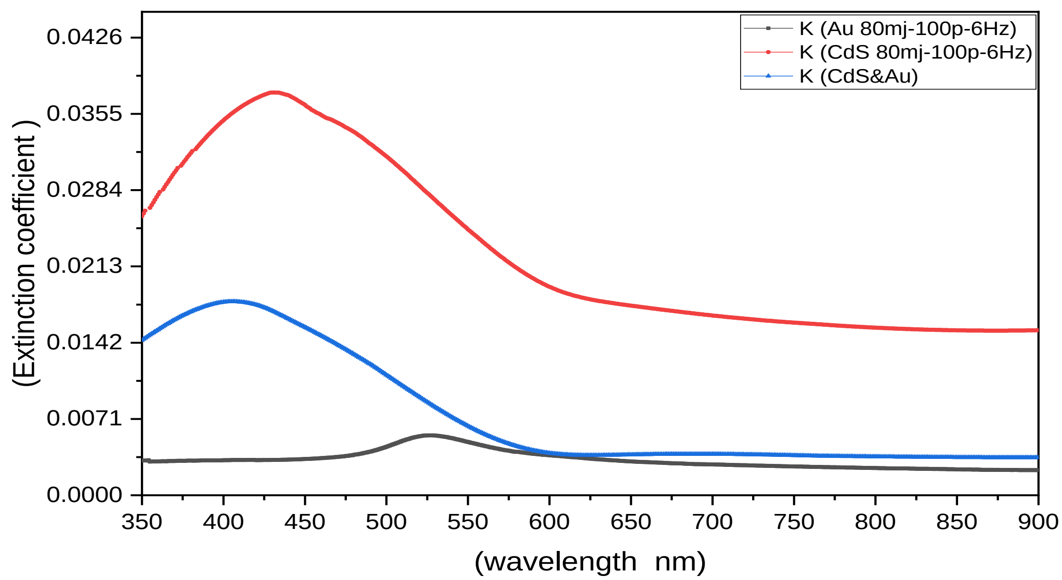

Figure 11: Shows the spectrum of the Extinction coefficient of gold and cadmium sulfate

- **Refractive index**

The refractive index is a crucial parameter in thin film optics. It signifies the ratio between the speed of light in a vacuum and its speed within the prepared films itself. As Figure 12 illustrates, the refractive index of the films varies depending on the incident light's wavelength (350-550 nm). This variation is likely due to the material's response to different light frequencies. Interestingly, Table 4 showcases how the refractive index changes with the composition of the film. Gold (Au) exhibits a high refractive index, causing significant light bending, while its absorption is relatively low. Conversely, Cadmium Sulfide (CdS) has a stronger light absorption, particularly at shorter wavelengths, and a high refractive index. The most intriguing finding lies in the CdS/Au composite. This combination not only boasts the highest absorption coefficient but also possesses the highest refractive index. This suggests a stronger light interaction and potential for manipulating light propagation. Evidently, combining materials strategically in thin films allows for tailoring their optical properties, paving the way for advancements in photovoltaics and light-based devices.

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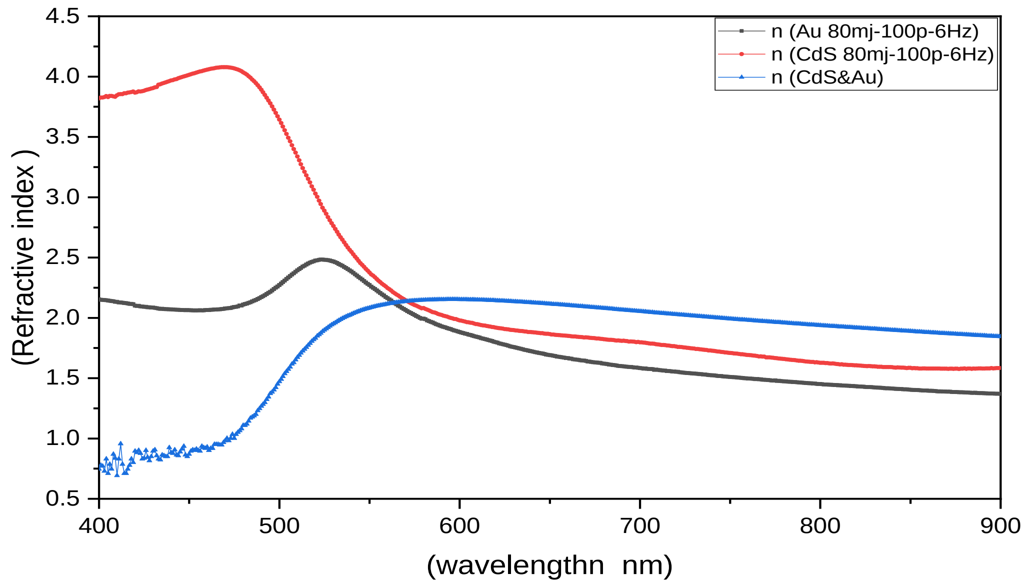

Figure 12: Shows the Refractive index spectrum of gold and cadmium sulfate

Table 4. shows the Absorption coefficient and Extinction coefficient and Refractive index for (CdS/Au)

Thin film	α cm-1	λnm	K	λnm	N	Λnm
CdS	*25.130*	*3.540*	*1.280*	*(100)*		*6.36*
Au	1100	535	0.0033	528	2.2973	224
CdS	*5950*	*398*	*0.0175*	*400*	*2.4831*	*523*
CdS / Au	11100	437	0.0375	433	4.1524	500

- **The Optical Energy Gap**

The optical energy gap (Eg) is calculated by adopting the Tauss equation according to the type of optical transitions that occur.

- **Direct Energy Gap Calculation**

The value of the energy gap for the allowed direct transmission is calculated by taking the value of the constant (r) equal to 1/2 in the Tauss equation, and thus the form of the equation is as follows:

$$\alpha h\nu \ = \ B\ (h\nu - Eg\ )^\wedge(\ 1/2)$$

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Then we plot the relationship between (αhν)2 versus the photon energy (hν), choose the straight part of the curve, and draw a straight line tangent to it that cuts the x-axis as the value of the optical energy gap for direct transmission corresponding to (Eg)^opt) is determined, as it shows that figure (13) is the optical energy gap values for the allowed direct transmission at room temperature.

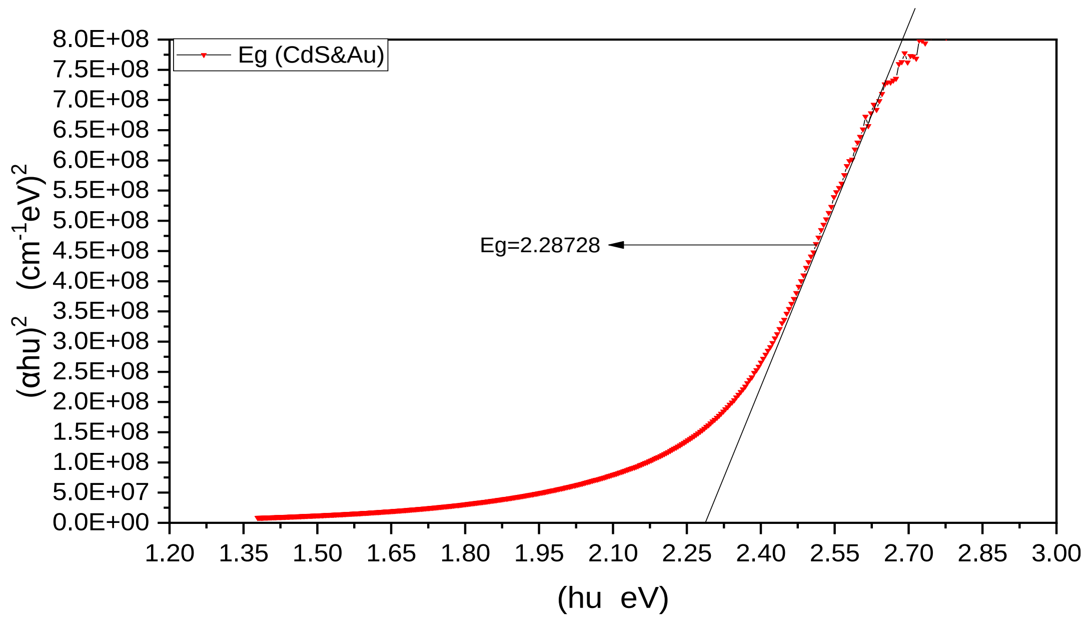

Figure 13. Shows the direct Energy Gap between Gold and Cadmium Sulfate

- **Indirect energy gap**

As for what we notice here, it is that the optical energy gap in which transitions are indirect, and this is what we notice as the value of the optical absorption coefficient indicates that its value is less than 104, as we notice in figure (14).

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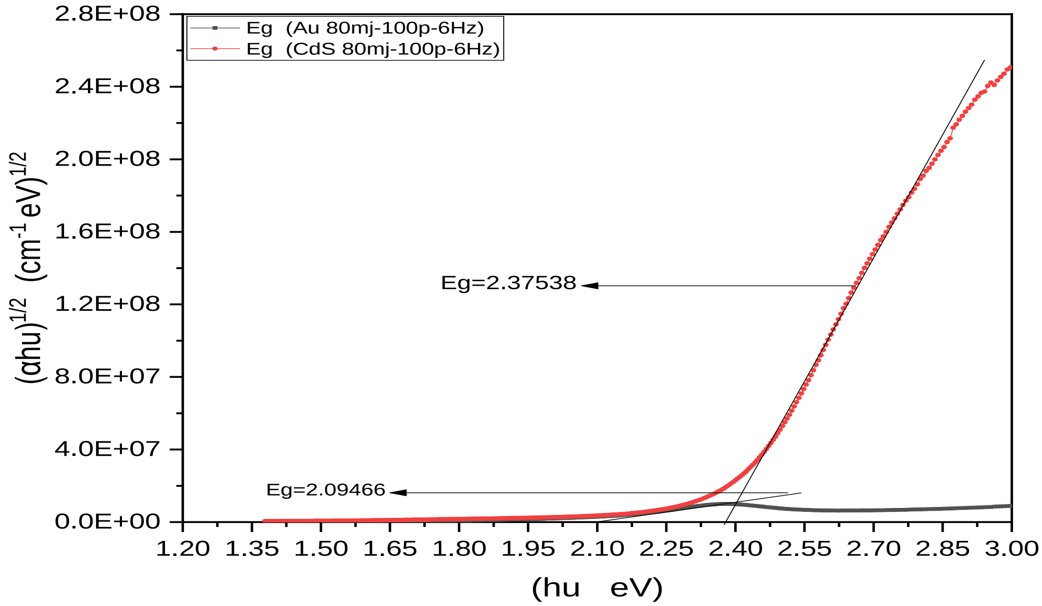

Figure 14. Shows the indirect Energy Gap of Gold and Cadmium Sulfate.

Table (5) showcases the estimated band gap energies for Au, CdS, and CdS/Au thin films. Both Au and CdS exhibit higher direct band gaps (2.09 eV and 2.37 eV respectively) compared to their indirect gaps. Interestingly, the CdS/Au composite has a direct band gap (2.28 eV) that falls between the individual values, suggesting its electronic properties are influenced by both materials.

Table 5. Direct and indirect optical energy gap for (CdS /Au)

Thin film	Indirect (Eg)	Direct (Eg)
Au	*2.09*	/
CdS	*2.37*	/
CdS /Au	/	*2.28*

- **Application**

After completing the manufacturing process of a solar cell using CdS and Au materials on p-type silicon, the film was examined and its Hall effect was found to be of n-type. This resulted in a change in the current generated by the cell. In order to determine the electrical characteristics of the films, the current-voltage characteristics were studied as shown in Figure 15.

In the case of darkness, the film exhibited good rectification behavior and a developed correlation. The dark current increased with the applied voltage. On the other hand, under reverse bias, the electric current showed a clear dependence. In the presence of light, the reverse current increased significantly with higher incident intensity during the cell examination process.

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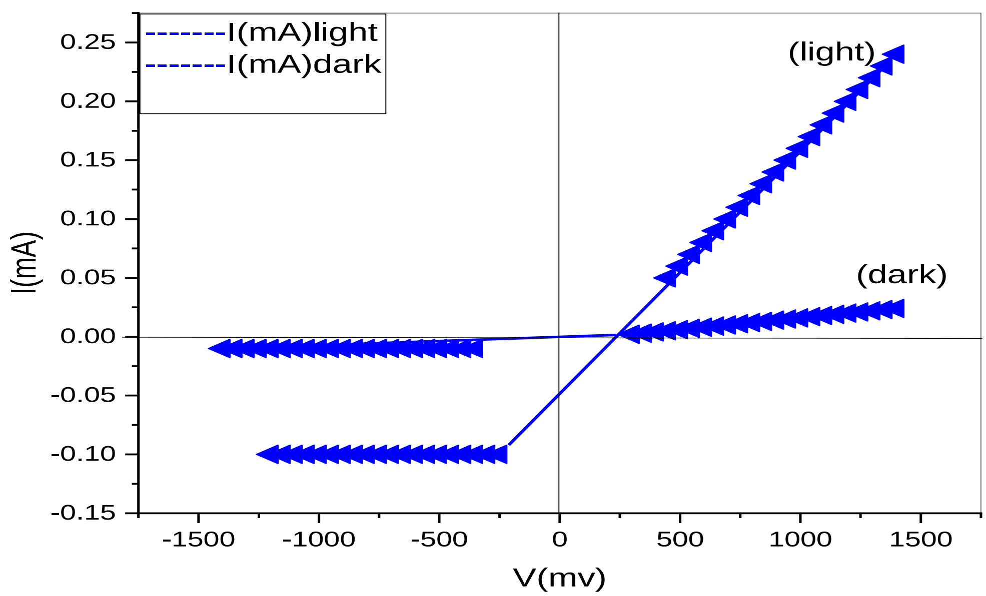

Figure 15: shows the dark current and light current for a silicon membrane prepared from CdS /Au.

CONCLUSIONS

The I and V values of the prepared solar cell increase with the increase of the layers of thin films on the surface of the solar cell, thus increasing the lighting current, as direct energy transfer occurs. The X-ray examinations of the films prepared by the pulsed laser deposition method showed that they have a polycrystalline structure and a hexagonal lattice, and the surface roughness decreases with the decrease of the concentration and by taking the threshold limit for each material.

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Conflict of interests.

There are non-conflicts of interest

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الخلاصة

المقدمة: أكدت دراسات عديدة أهمية عملية تصنيع الخلايا الشمسية والكواشف الضوئية وكذلك المتحسسات بانواعها لان لها اهمية في اغلب جوانب الحياة العملية حيث تدخل في صناعات عديدة لذا تم العمل عليها ودراستها

طرق العمل: تم استخدام مادتي الذهب(فلز) وكذلك كبريتات الكادميوم والتي كانت على شكل باودر تم كبسها بضغط (15 ميكا باسكال) على شكل قرص قطره (2سم) وتم استخدام تقنية (PLD) لتكوين الاغشية الرقيقة حيث تم التغير في عدد النبضات وتم تثبيت قدرة الليزر 100ملي جول واستخدام طول موجي 1064 نانو متر.

النتائج:

اظهر غشاء Au/CdS بنية متعددة البلورات ذات شبيكة سداسية،ان وجود الذهب في مادة CdS ادى إلى إجهاد شبيكي منخفض للغاية، حيث أن الأقطار الذرية لـ (0.154) CdS نانومتر والذهب (0.165) نانومتر.

الاستنتاجات:

اظهرت الدراسة الحالية امكانية تصنيع أغشية Au/CdS بطريقة الانتشار الحراري .ان قيم التيار والفولتية للخلية الشمسية المحضرة تزداد بزيادة طبقات الأغشية الرقيقة على سطح الخلية الشمسية وبالتالي يزداد تيار الإضاءة حيث يحدث انتقال مباشر للطاقة. اظهرت فحوصات الأشعة السينية للأغشية المحضرة بطريقة الترسيب بالليزر النبضي انها ذات بنية متعددة البلورات وشكلها سداسي وان الأغشية المحضرة في حالة CdS-Au وان حجم حبيبات الأغشية الرقيقة يزداد بزيادة طاقة الليزر وعدد النبضات و كذلك نلاحظ ان خشونة السطح تقل بتقليل التركيز.

الكلمات المفتاحية: الترسيب، الجسيمات النانوية، الخلايا الشمسية، التحليل الطيفي المرئي، أجهزة استشعار الغاز.