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Investigation On The Influence of Varying Substrate Temperature On The Physical Features of Yttrium Doped Cadmium Selenide Thin Films Materials

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Abstract

The influence of varying substrate temperature on the structural, morphological, optical, and electrical properties of yttrium doped CdSe using the spray pyrolysis deposition method is reported in this work. The synthesized thin materials were characterized using X-ray diffraction-XRD, Scanning electron microscopy (SEM), Energy dispersive X-Ray (EDX), UV-Spectrophotometer, and Four-point probe. The XRD analysis revealed a polycrystalline hexagonal structure with the most preferred orientation along (100) plane for all the films irrespective of the substrate temperature. Y: CdSe deposited at 160°C gave the best crystallinity. The surface morphology ascertained using SEM shows uniform, well dense, and agglomerated films. The as-deposited films were homogenous devoid of cracks suggesting uniform deposition. The EDX results show the presence of the major elements i.e. Cd, Se, and Y which confirms the formation of CdSe and novel YCdSe thin particles. The optical results reveal that Y: CdSe deposited at 180°C exhibited better optical property when compared to other films with an energy bandgap value of 1.50eV. The electrical studies show that an increase in substrate temperature of the thin material decreases the resistivity with increasing thickness and increasing conductivity which reveals that the films are semiconducting material good for use in electronic and optoelectronic applications and more so for photovoltaic applications due to the narrowed bandgap.

Keywords: *Y- doped CdSe, substrate temperature, XRD, SEM, bandgap, optoelectronics*

I. Introduction

Cadmium-selenide (CdSe) is an II-VI group compound semiconductor material, crystallizing in either the zinc blende or wurtzite structure [1], [2]. Its excellent performance and suitable properties such as bandgap, high absorption coefficient, and high photosensitivity make it useful in optoelectronic and electronic applications, such as nano-sensors, laser diodes, high-efficiency solar cells, γ-ray detectors, and devices for biomedical imaging [3], [4], [5]. CdSe has a direct bandgap and high absorption coefficient close to the band edge, making it suitable for use in thin-film devices; it is mainly interesting for its applications in hybrid solar systems [6]. CdSe thin materials have been synthesized by many researchers via various film deposition techniques, such as spray pyrolysis [7], SILAR [8], Electrodeposition [9], Electron beam evaporation [10], chemical bath deposition (CBD) [11], [1], etc. More so, to increase the performance of CdSe nanocrystalline thin films, many researcher used the dopant impurities and made thin film of CdSe:Fe [12], [13], CdSe:Cr [5] , CdSe:Zn [14], CdSe:Cu [15], [16], CdSe:Ni [17] and CdSe:Mn [18],[19] etc. To the best of our knowledge, CdSe doped with yttrium has not to be synthesized. Therefore in this study, we reported the synthesis of yttrium Copper selenide (YCuSe) semiconductor thin material using spray pyrolysis technique and the effect of substrate temperature on the structural, morphological, optical, and electrical properties of the deposited thin materials for electronics, optoelectronics, and photovoltaic purposes.

II. Materials and Method

The chemical used comprises Cadmium Sulphate hydrate ($CdSO_4.8H_2O$), Selenium (IV) Oxide (SeO_2), Hydrogen chloride (HCl), and Yttrium (Y). Finally, the spray-pyrolysis method was employed as the deposition techni

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A. Substrate preparing

An ordinary soda-lime glass was used as a substrate. The glass slides were immersed in methanol/acetone and later ultrasonicated for 30minutes after which they were thoroughly rinsed in deionized water and dried in an oven.

B. Preparation of Solutions

0.01 mol solution of $CdSO_4.8H_2O$ was prepared by dissolving 1.248 g/mol of it in 500 ml of deionized water. 0.01 mol. solution of selenium (IV) Oxide was prepared by dissolving 3.158 g with 5 ml of Hydrogen chloride (HCl) with 100 ml of deionized water. The deposition bath system is composed of a source of cation (i.e $CdSO_4.8H_2O$ - Cd^{2+}), a source of the anion (i.e SeO_2 - Se^{2-}), 0.1mol% of Yttrium, deionized water all in 500/100 ml beaker, the magnetic stirrer was used to stir the reaction bath.

C. Spray process/procedure

The spray process involves the optimization of several process parameters. The values of the optimized process parameters are Precursor flow rate 0.07 ml/min, precursor CdSe, Spray nozzle to substrate distance: 8 mm, Spray-nozzle specification: internal diameter 0.16 mm, outside diameter: 0.32 mm. Substrate temperature 400°C, and Atomizing voltage 3.5KV. Electrostatic atomization is used in this technique. The substrate was attached to the substrate holder, with the temperature regulator; the temperature was varied from 140°C, 160°C, 180°C, and 200°C. The precursor ion was pumped through the pump directly to the nozzle. As the mixture passes through the nozzle and strikes the surface of the substrate, evaporation of the residual solvent takes place thereby spreading the droplet, and then the salt decomposes. Finally, CdSe is deposited on the substrate. Film uniformity is ensured by moving both the nozzle (needle) and the substrate. This process is repeated with a constant dopant concentration of 0.1mol% of yttrium (Y) at different substrate temperatures as summarized in Table 1.

Table 1: Deposition parameters of CdSe and YCdSe at varied substrate temperature.

Samples	**$CdSO_4.8H_2O$ (mI)**	**SeO_2 (ml)**	**Yttrium (ml)**	**Voltages (KV)**	**Temperature (Degree)**
CD	20	10		3.5	120
CDY **(140°C)**	20	10	5	3.5	140
CDY **(160°C)**	20	10	5	3.5	160
CDY **(180°C)**	20	10	5	3.5	180
CDY **(200°C)**	20	10	5	3.5	200

D. Characterization of the thin materials

The fabricated films were analyzed using X-ray diffraction-XRD, Scanning electron microscope-SEM, Energy dispersive X-ray Analysis-EDX, UV-1800 visible spectrophotometer, and old Jandel four-point probes technique (model T345) for structural studies, film morphology, identification of the major elemental composition, optical characterization, film thickness, and electrical properties respectively. More so, other properties required for better evaluation of these deposited thin materials were ascertained using appropriate mathematical equations.

III. Results and Discussion

A. XRD result of pure and Y doped CdSe at a different substrate temperature

The XRD pattern of pure and Y doped CdSe thin materials deposited at different substrate temperatures (140°c to 200°C) are displayed in figure 1. Four clearly defined peaks corresponding to crystal plane (100), (102), (200), and (210) were noted. The XRD analysis reveals that the samples are polycrystalline, having hexagonal structure and with the most preferred orientation along (100) plane irrespective of the substrate temperature. Variation in substrate temperature was observed to affect the crystallinity of films. An increase in substrate temperature increases the intensity of the peak up to 160°C which then decreases with a further increase in substrate temperature. From the record Y: CdSe deposited at 160°C gave the best crystallinity based on the intensity value and having the most prominent peaks. This result corresponds to that of Yadav *et al.,* [7] for CdSe thin films deposited at different substrate temperatures via spray pyrolysis technique. To the best of our knowledge, there is no published information on the structural properties of Y: CdSe. Sivasankar *et al.,* [5] also reported a similar result where a hexagonal structure was obtained for pure and Cr doped CdSe samples deposited via a solid-state reaction method. The data gotten during XRD analysis was used in evaluating some structural parameters [6], [20] as outlined in table 2.

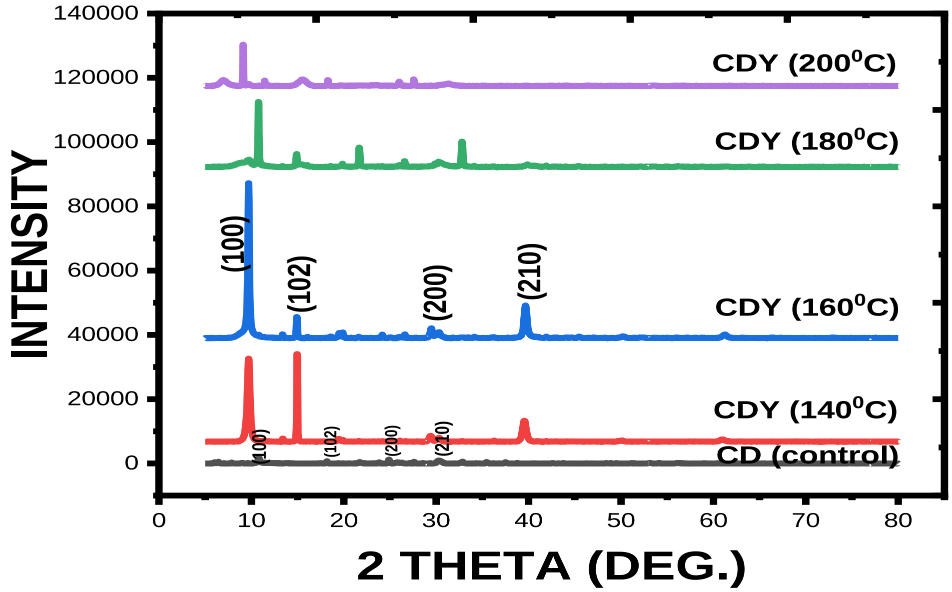

Figure 1: XRD pattern of pure and yttrium-doped CdSe at a different substrate temperature

Table 2: Structural values for the pure and Yttrium-doped CdSe at different temperatures.

Sample	2θ (degree)	Spacing d(Å)	Lattice constant (Å)	FWHM, β	Hkl	Crystallite Size,D (nm)	Dislocation density, δ m^2
CD-CdSe	9.5290	9.27277	16.06091	0.18517	100	0.75139	5.37038
CDY-140⁰C	14.9501	5.92032	11.84063	0.20958	102	0.667252	6.82167
CDY-160⁰C	19.8909	4.45949	8.918985	0.14899	200	0.951148	3.3576
CDY-180⁰C	29.4979	3.02533	6.764852	0.22584	210	0.634872	7.46563
CDY-200⁰C	39.7912	2.26326	5.543833	0.22499	300	0.655395	7.03276

B. SEM and EDX results

The pictorial SEM images and EDX spectrum of pure and Y doped CdSe deposited at the substrate temperature of 140°C are displayed in fig. 2(a-b) and fig. 3(a-b) sequentially. The surface morphology of these thin films investigated using scanning electron microscopy (SEM) shows uniform, well dense, and agglomerated films. The as-deposited films were homogenous devoid of cracks suggesting uniform deposition. This characteristic implies that these film cells will serve as a good material for use in electronic industries and photovoltaic applications [21]. The addition of yttrium dopant was observed to increase the grain size. The elemental composition analysis of the pure and Y doped CdSe thin materials was actualized using the EDX technique. The EDX spectrum results are depicted in fig. 3a and 3b supports the film composition with the presents of the major elements-Cu, Se and Y.

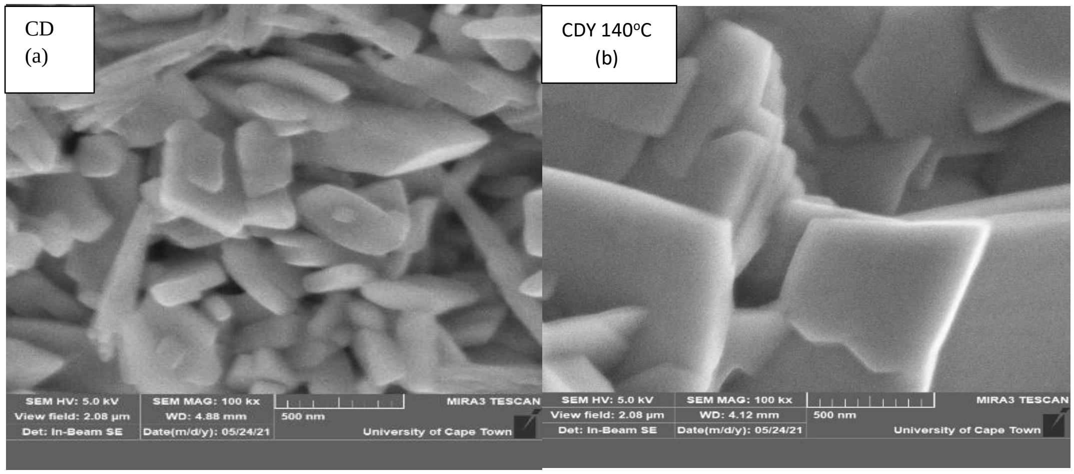

Fig 2. Pictorial SEM images of (a) pure and (b) Y doped CdSe at substrate temperature of 140°C

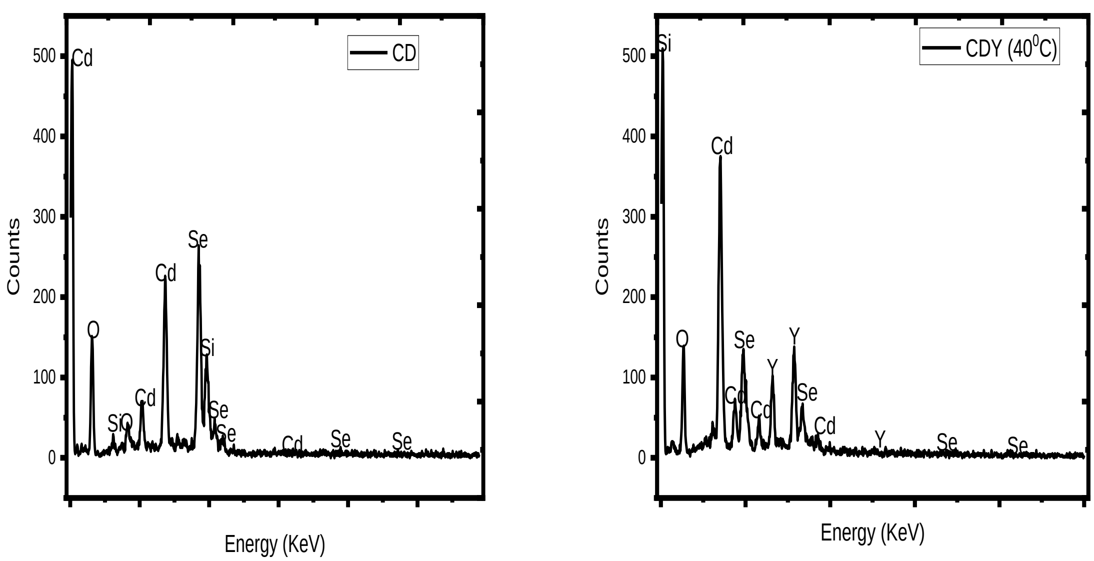

Fig 3. EDX spectrum of (a) pure and (b) Y doped CdSe at the substrate temperature of 140°C

C. Optical and Solid-state result of pure and Y-doped Cd Se thin material

The absorbance of pure and Y- Y-doped cadmium selenide (Y: CdSe) thin films at different substrate temperatures as a function of wavelength is presented in fig 4a. The absorbance spectral of all the samples vary with the wavelength, in the same way, decreasing gradually with an increase in wavelength but no particular trend with substrate temperature. The maximum absorbance for all the samples occurred in the UV region with sample grown at the substrate temperature of 180°C having the highest absorbance value of 0.88 amidst the other samples grown at 140°C, 160°C, and 200°C with 0.78, 0.65, and 0.40 as their maximum respectively at 300nm. The pure CdSe which acts as the control was observed to record the least absorbance value.

This implies that the introduction of Y dopant to pure CdSe enhances its absorbance strength.

The transmittance of Yttrium doped cadmium selenide (Y/CdSe) thin films at different substrate temperatures as a function of wavelength is presented in fig 4b. The transmittance spectral of all the samples varies with the wavelength, in the same way, increasing gradually with an increase in wavelength but no particular trend with substrate temperature. The average transmittance in the ultra-violent region for all the samples is in the range of 16% to 50% which increased to a maximum average of 30% to 70% in the infra-red region with sample grown at the substrate temperature of 160ºC having the highest transmittance value. Our findings follow a similar trend as reported by Rani et al [10] for Electron-beam deposited CdSe doped with Zn and also in line with Jasmi [22] for CdSe prepared by chemical reaction.

The reflectance of Y-doped cadmium selenide (Y: CdSe) thin films at different substrate temperatures as a function of wavelength is revealed in fig 4c. Generally, all the samples exhibited very weak reflectance in all the electromagnetic regions. It was also observed from the graph shown in figure 4c that the reflectance of CdSe samples grown on substrate temperatures of 140ºC, 180ºC, and 200ºC tend to increase with an increase in wavelength except for CdSe grown on substrate temperature of 160ºC which decreases with an increase in wavelength. For all the samples a least and maximum value of 0.03 and 0.21 was obtained in the Uv and Vis respectively which makes the samples a potential material for use in the fabrication of solar cells as an anti-reflector [23].

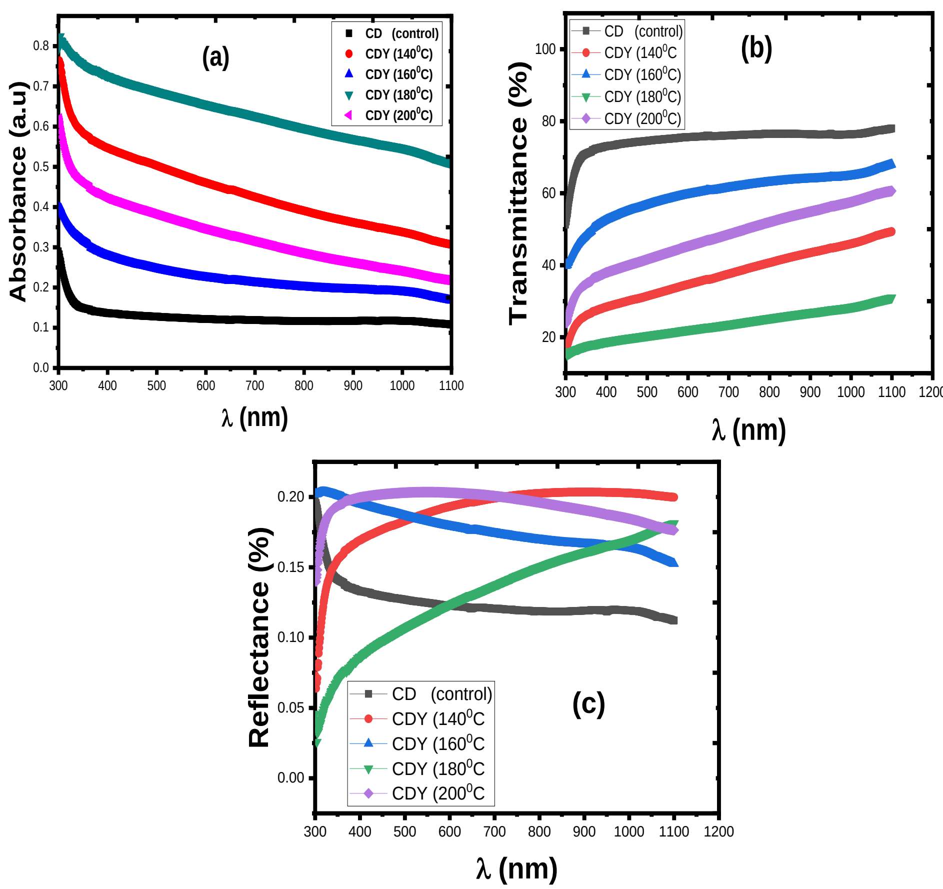

Fig. 4: (a) Absorbance spectral (b) Transmittance spectral and (c) Reflectance spectral of pure and Y/CdSe thin materials deposited at different substrate temperature

D. Energy band gap (E_g)

The relationship between $(\alpha h\nu)^2$ and photon energy for pure and Y-doped cadmium selenide (Y: CdSe) thin films at different substrate temperatures is shown in fig 5 and the energy bandgap for the materials were gotten from the plot. From the plot, it can be observed that the energy bandgap values of the Y: CdSe thin materials range from 1.50 eV to 1.76 eV depending on the substrate temperature and the summary is also shown in fig 5. The pure CdSe which acts as control was observed to record the highest energy bang value of 1.85eV. We can conclude that the introduction of Y dopant narrowed the energy gap of pure CdSe thereby making it a better material for use in photovoltaic applications.

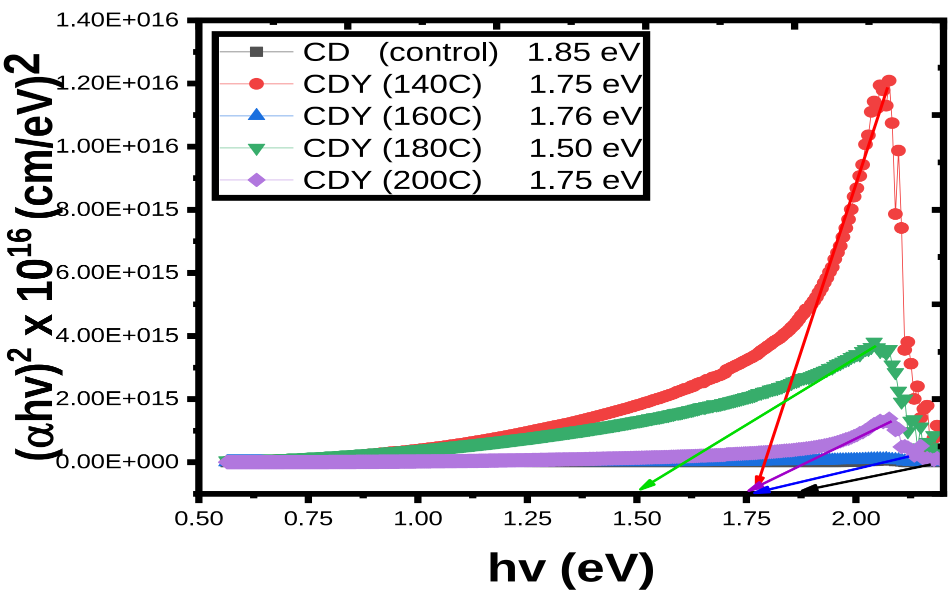

Fig. 5: Plots of $(\alpha h\nu)^2$ against hν for pure and Y-doped CdSe thin material at different substrate temperature

Figure 6a reveals the variation of extinction coefficient as a function of photon energy for pure and Y-doped CdSe at different substrate temperatures varying in the range of 140ºC – 200ºC. The result indicates that the value of extinction coefficient attained a maximum at high photon energy except for the Y: CdSe sample deposited at the substrate temperature of 180ºC which decreases drastically as the photon energy increases. Generally, it was observed that an increase in the substrate temperature reduced the extinction coefficient of Y: CdSe. From the spectra Y: CdSe deposited at 140ºC has the highest extinction coefficient which shows it is a propitious material for use in thin-film solar cell fabrication [25].

Figure 6b reveals the variation of refractive index as a function of photon energy for pure and Y-doped CdSe at different substrate temperatures varying in the range of 140ºC – 200ºC. It was noticed from the plot that the refractive index of the thin materials didn't follow a particular trend, Y: CdSe samples deposited on a substrate of 140ºC and 180ºC decreases drastically while samples deposited on a substrate of 160ºC and 200ºC increases slightly as the photon energy increases.

The Plot of optical conductivity against hv for pure and Y: CuSe thin materials deposited at different substrate temperatures (140ºC to 200ºC) is displayed in fig 6c. The optical conductivity of all the samples was seen to increase with increases in photon energy despite the variation in substrate temperature. More so, Y: CuSe film deposited at a substrate temperature of 160ºC and 140ºC was observe to record the highest and lowest optical conductivity value. For a typical semiconductor, the optical conductivity increases for higher photon energy which agrees with the result obtained in this study [23].

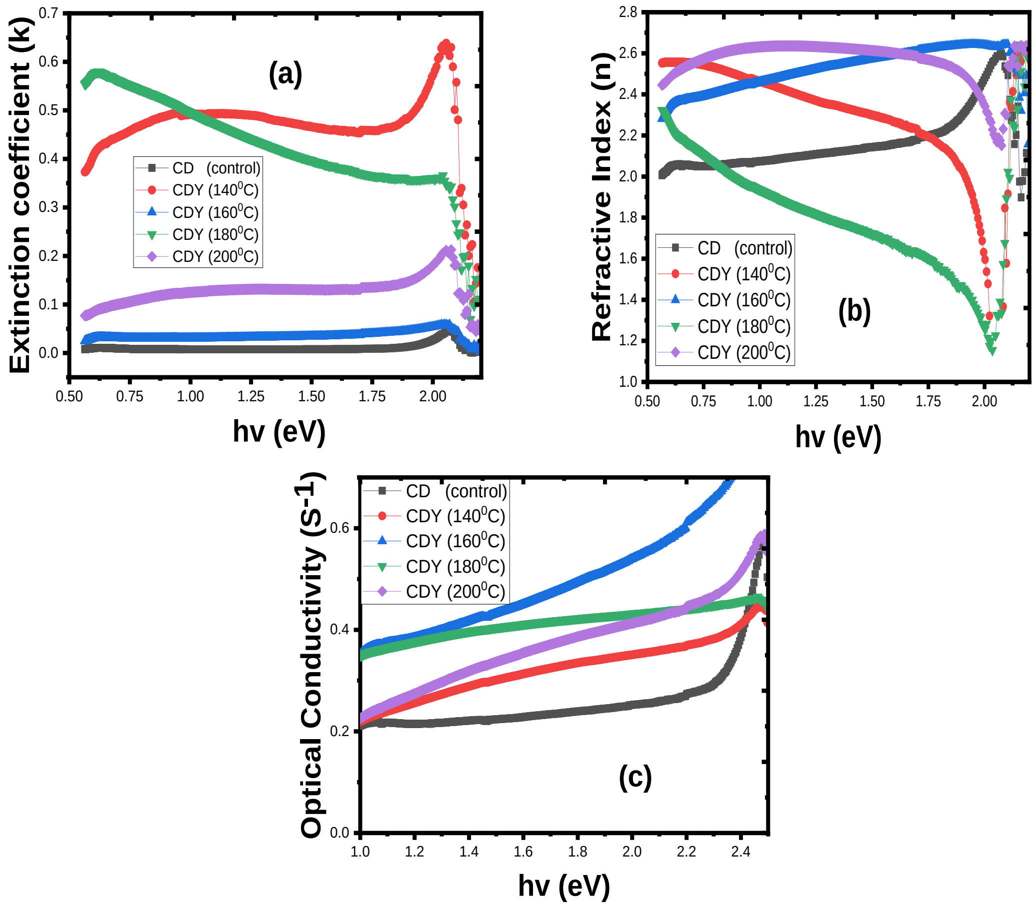

Fig. 6: Variation of (a) Extinction coefficient (b) refractive index and (c) Optical conductivity with photon energy for pure and Y doped CdSe thin materials deposited at a different substrate temperature

The plots of real and imaginary dielectric constant against photon energy for pure and Y-doped CdSe grown at different substrate temperature is displayed in fig 7(a-b) respectively. Figure 7a which depicts the plot of real dielectric constant against photon energy reveals that the Y/CdSe samples deposited at different substrate temperatures (140 to 200°C) followed no particular trend, as the photon energy increases the samples deposited at 140°C and 180°C decreases drastically while samples deposited at 160°C and 200°C increases gradually. A peak value of approximately 7.01 was recorded for samples grown at substrate temperatures of 160°C and 200°C between photon energy of 1.0 and 2.0 eV. On the other hand, the imaginary dielectric constant depicted in fig 7b shows a similar trend as seen in the real dielectric part, as the photon energy increases the samples deposited at 140°C and 180oC decreases drastically while samples deposited at 160°C and 200°C increases slightly.

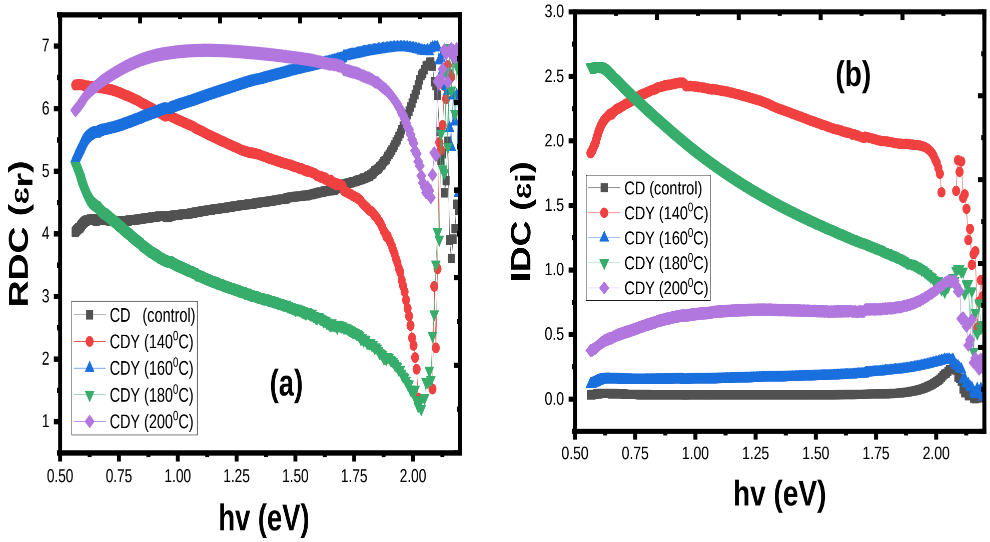

Fig.7: Plots of (a) real and (b) imaginary dielectric constant against photon energy for pure and Y-doped CdSe grown at a different substrate temperature

E. Electrical properties of pure and Y doped CuSe (at different substrate temperatures) thin materials

The thickness, resistivity, and conductivity values of pure and Y doped CdSe (Y:0.1mol%) grown at different substrate temperatures are summarized in table 3 while figure 8 illustrates the relationship between resistivity and conductivity with the film thickness of Y: CdSe thin materials. The result reveals the dependencies of resistivity and thickness on the substrate temperature. As the substrate temperature of the material increases from 140ºC to 200ºC the resistivity of the material decreases with increasing thickness of 150.21nm to 161.13nm and increasing conductivity values which is one of the features of a typical semiconductor [25].

Table 3: Electrical properties of CdSe and CdSe/Y (at different substrate temperatures)

Samples	Thickness, t (nm)	Resistivity, **ρ** (Ω.m)	Conductivity, **σ** $(\Omega.m)^{-1}$
CD control	150.21	6.210×10^{-6}	1.610×10^{5}
CDY 140^0C	152.32	7.427×10^{-6}	1.346×10^{5}
CDY 160^0C	156.41	7.456×10^{-6}	1.341×10^{5}
CDY 180^0C	157.21	7.359×10^{-6}	1.358×10^{5}
CDY 200^0C	161.13	7.327×10^{-6}	1.364×10^{5}

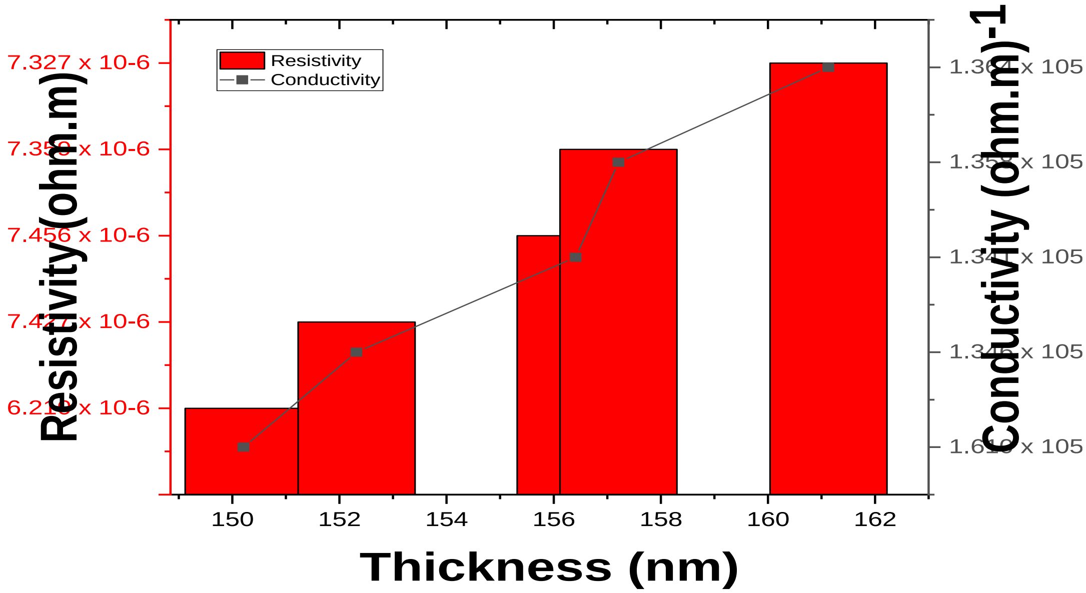

Fig. 8: A bar chart like comparison of resistivity and conductivity of Y doped CdSe (at different substrate temperatures) with film thickness.

IV. CONCLUSION

The spray pyrolysis deposition method has been successfully employed to synthesize Undoped and Y-doped CdSe (0.1mol%) with varying substrate temperatures (140°C – 200°C). The effect of the yttrium doping and substrate temperature variation on the structural, morphological, electrical, and optical properties of CdSe and Y: CdSe is reported in this research work. The XRD analysis revealed a polycrystalline hexagonal structure with the most preferred orientation along (100) plane for all the films irrespective of the substrate temperature. From the result, Y: CdSe deposited at 160°C gave the best crystallinity based on the intensity value and having the most prominent peaks. The surface morphology ascertained using SEM shows uniform, well dense, and agglomerated films. The as-deposited films were homogenous devoid of cracks suggesting uniform deposition. The EDX results show the presence of the major elements i.e. Cd, Se, and Y which confirms the formation of CdSe and novel YCdSe thin particles. For the electrical studies, the result shows that an increase in substrate temperature of the thin material decreases the resistivity with increasing thickness and increasing conductivity which reveals that the films are semiconducting. The energy bandgap values of the Y: CdSe thin materials range from 1.50 eV to 1.76 eV depending on the substrate temperature while the pure CdSe which acts as control was observed to record the highest energy bang value of 1.85eV. It was also observed that Y: CdSe deposited at 180°C gave a better optical property when compared to other films with an energy bandgap value of 1.50eV. Thus the narrowed energy bandgap, improved crystallinity, and high conductivity displayed by Y: CdSe makes it a better material for use in photovoltaic, electronic, and optoelectronics applications.

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