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Growth and optimization of physical properties of cadmium selenide semiconductor material via yttrium doping for photovoltaic/solar energy purposes

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Abstract

The synthesis and analysis of cadmium selenide and yttrium doped cadmium (YCdSe) materials at different dopant concentrations (0.01, 0.02, 0.03, and 0.04 mol%) via spray pyrolysis technique (SPT). The influence of Y-incorporation and variation on the morphology, elemental composition, electrical, structural, and optical features of CdSe were analyzed via SEM, EDX, four-point probe, XRD, and UV-vis spectrophotometry respectively. The SEM image of Y-doped CdSe (0.01 and 0.04 mol%) is significantly different from the undoped. The EDX spectrum result confirms the growth of pure and Y-CdSe thin materials. The XRD patterns revealed that all the synthesized thin materials are polycrystalline films that possess a hexagonal structure with the predilect orientation and highest intensity along the (100) plane. The incorporation of yttrium dopant was noticed to enhances the crystallinity of CdSe. An increase in Y-concentration from 0 to 0.04 mol%, led to a decrease in the resistivity of CdSe with decreasing film thickness and increasing conductivity value. The energy bandgap of 1.71 eV for cadmium selenide and 1.41 – 1.61 eV for Y-doped. The general result shows that novel YCdSe thin materials possess better and improved features for the production of photovoltaic cells when compared to the undoped ones.

1. Introduction

Semiconductor materials are normally small bandgap insulators. The coaction of semi-conductors with photons is of importance for photovoltaic and optoelectronic devices among other things for the analysis of semi-conductor furnishing. When a light strikes a semi-conductor, reflection, transmission, and absorption are studied [1]. The reception of the semi-conductor mostly relies on the photon energy of the light and different technique add to the dielectric function. For the photon energy to be fixed proficiently it must exceed the energy band-gap of the semiconductor material in question [2]. In recent times, several research works have been put in to enhance semiconductor's efficiency using doping and coupling of these elements. Doping rare earth nanoparticles have earned extremely attention for their colossal photo-catalytic activities in the breakdown of biological contaminants due to a large number of oxygen vacancies, inhibition of electron-hole recombination, and firm saturation of hydroxide ions on the exterior segment of the catalyst [3]. Due to their deep diffusivity, which are known to perform important functions such as gloomy and implementing the circus factor in dielectric materials [4]. One of the promising dopants in the family of sporadic earth resources is Yttrium (Y3+). This is because it enhances fatigue endurance, leakage current, and remanent polarization [5]. Yttrium as well performs as an acceptor or donor ion. Alternatively, the important effect of yttrium doping is the modification in the conductivity feature of the doped material in connection to its doping site.

CdSe is a semiconducting material that belongs to group II-IV in the periodic table [6]. It crystallizes either as a zinc blende or wurtzite structure and exhibits excellent performance [7], [8]. It also possesses suitable features such as a bandgap, high photosensitivity, and high absorption coefficient which makes it advantageous in electronic, photovoltaic, and optoelectronic applications, such as increased productivity solar cells, X-ray detectors, laser diodes, and devices for biomedical imaging [9]- [10]. sCadmium selenide thin materials have been fabricated using different material deposition techniques, such as CBD, SILAR, Spray pyrolysis, Electron beam evaporation, Electrodeposition [7], [11]-[15]. More so, to optimize the effectiveness of CdSe thin materials, a good number of researchers have worked on CdSe doped compounds such CdSe:Cr [10], CdSe:Fe [16], [17] CdSe:Zn [18], CdSe:Ni [19], CdSe:Cu [20], [21], CdSe:Mn [22], [23] and CdSe:Sm [24] etc. However, we observed that there is no scientific record on CdSe:Y thus far. In this current research, the growth and characterization of Y-doped CdSe thin materials have been studied and analyzed.

Experimental details

In this study, the spray pyrolysis deposition technique was used for the growth of thin materials. It is primarily a chemical growth technique that involves spraying thin droplets of the required thin material onto a pre-heated substrate. Via thermal-decomposition of the droplets onto the substrate continuous films are produced. CdSe and Y-doped CdSe (dopant molarity 0.01, 0.02, 0.03, and 0.04 mol%) thin materials were deposited onto a glass substrate via spray pyrolysis method. 0.01 M solution of Cadmium Sulphate hydrate ($CdSO_4.8H_2O$) was measured by dissolving 3.847 g/mol in 500 ml of distilled water. 0.01 M of selenium (IV) Oxide (SeO_2) was measured by dissolving 3.158 g/mol with 5 ml of Hydrogen chloride and 100 ml of distilled water. Yttrium (Y) concentration of 0.01, 0.02, 0.03, and 0.04 mol% were used as the dopant. The optical glass was utilized as the substrate and preceding the deposition these substrates were treated with methanol and acetone for 30mins, rinsed with deionized water, and oven-dried. The precursor spray rate was 0.07 ml/min at a constant substrate temperature of 400^{o}C, spray nozzle to substrate distance of 8mm, and atomizing voltage of 3.5 kV. The summary of the deposition parameters is shown in table 1. The as-deposited thin materials were characterized in other to ascertain the impact of Y dopant on the morphological, elemental compositional, structural, electrical, and optical features of CdSe using Scanning electron microscopy-SEM, Energy dispersive X-ray-EDX, X-ray diffraction-XRD, four-point probe, and Uv-Vis spectrophotometer respectively.

Table 1: Parameters for fabrication

Samples	$CdSO_4.8H_2O$ (ml)	SeO_2 (ml)	Yttrium (ml)	Voltages (KV)	Dopant conc. (Yttrium) (mol%)
CD	20	10		3.5	
CDY (0.01)	20	10	5	3.5	0.01
CDY (0.02)	20	10	5	3.5	0.02
CDY (0.03)	20	10	5	3.5	0.03
CDY (0.04)	20	10	5	3.5	0.04

3. Results and Discussion

3.1: Morphological and elemental compositional analysis

Scanning electron microscopy has been confirmed to be a peculiar, versatile, and suitable approach to study surface morphology and to ascertain the grain size of the materials. The SEM microstructure of CdSe and Y-doped CdSe (0.01 and 0.04 mol%) thin materials at 100 Kx magnification are shown in Fig 1(a-c). From the SEM result, it was observed that both the undoped and Y-doped CdSe films were uniform with dense surface morphology covering the whole substrate and without cracks. The grain size of undoped CdSe thin material was observed to be thinner upon the addition (fig.1(b)) and increase of the dopant (fig.1(c)). Fig 2(a-c) showed the EDX plot of cadmium selenide and YCdSe (0.01 & 0.04 mol%) materials. The EDX spectrum in fig 2(a) points out the deposition of pure CdSe while fig. 2(b) and (c) reveals the presence of Y in CdSe samples.

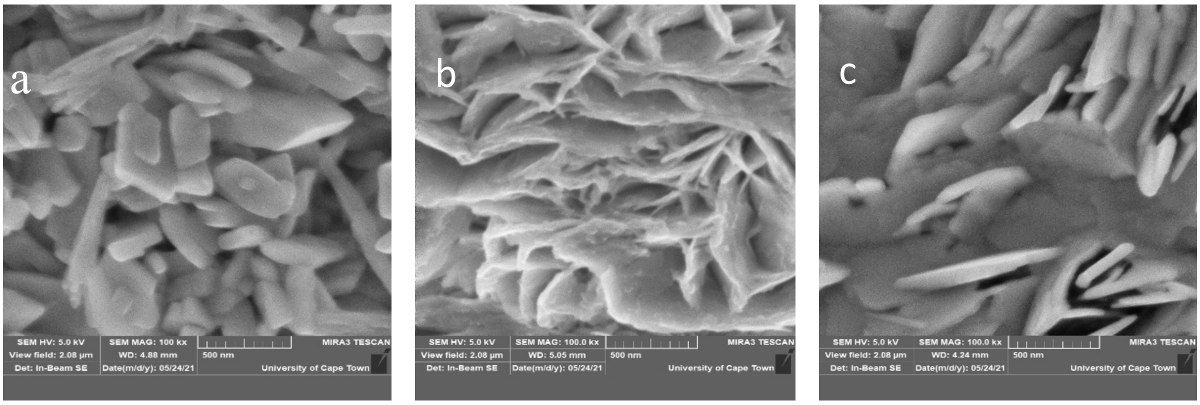

Fig.1: (a) SEM microstructure of CdSe; (b) YCoSe 0.01 mol%, and (c) YCoSe 0.04 mol%

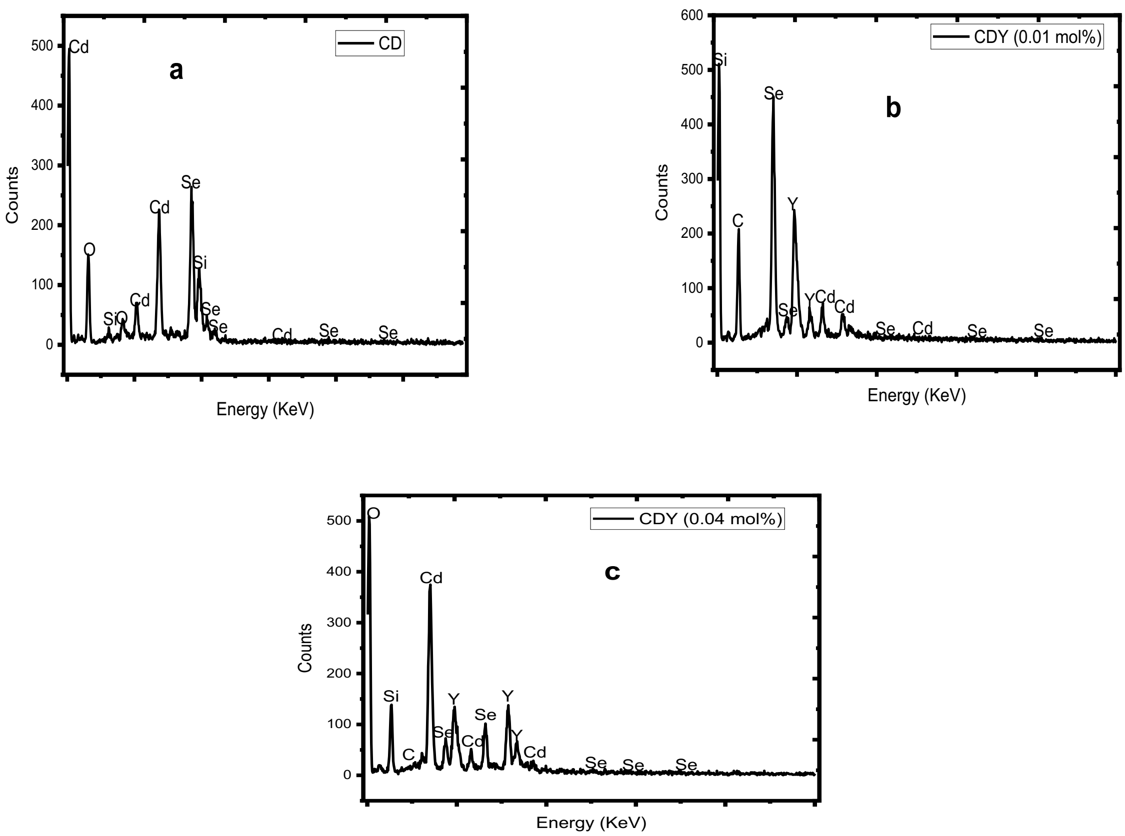

Fig 2. EDX spectrum of (a) CdSe (b) YCoSe 0.01 mol% (c) YCoSe 0.04 mol% materials

3.2: Structural result

Fig 3 displays the X-ray diffraction patterns of undoped and YCdSe materials deposited at different Y mol% concentrations. The XRD patterns reveal that the nature of all the deposited thin materials is polycrystalline possessing a hexagonal structure based on the observed and standard values for (hkl). The figure reveals the presence of (100), (102), (200), and (210) planes with the preferred orientation and highest intensity along the (100) plane. The incorporation of yttrium dopant was noticed to enhances the crystallinity of CdSe which was observed in the peak's intensity for all the YCdSe samples. Similar result was reported by Sivasankar *et al., 2017,* where a hexagonal structure was noticed for pure and Cr incorporated CdSe films prepared using a solid-state reaction technique. The XRD analysis data was used in the evaluation of some structural parameters as shown in table 2 [10], [25].

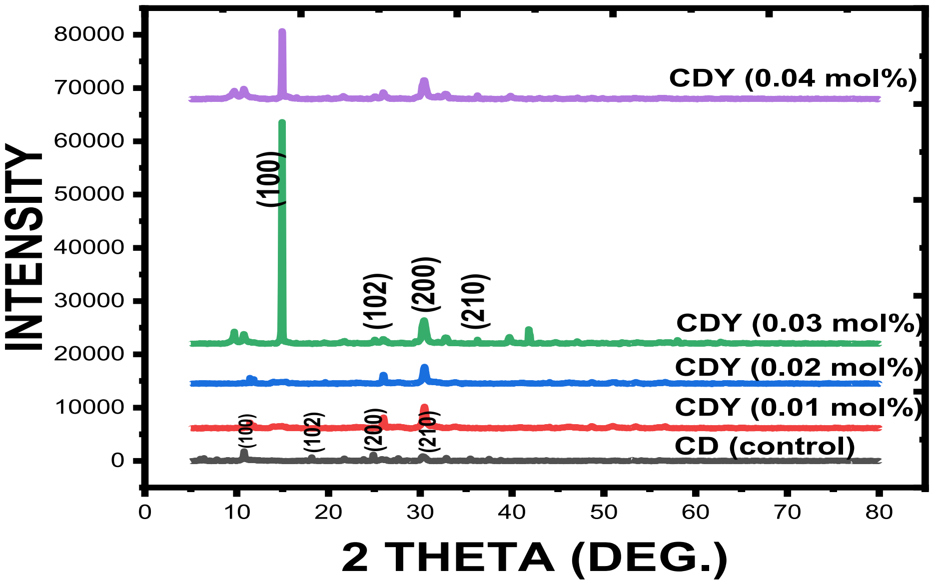

Fig. 3: XRD patterns of CdSe and YCdSe at various mol% concentrations

Table 2: XRD values for the CdSe and YCdSe at varying molar percentage dopant.

Label	2θ (degree)	Spacing d(Å)	Lattice constant (Å)	FWHM, β	Hkl	Crystallite Size, D (nm)	Dislocation density, δ m^2
CD-CdSe	10.7985	8.18638	14.17739	0.18474	100	0.752131	5.35981
	18.1753	4.87700	9.752760	0.20927	102	0.669992	6.76600
	24.9346	3.56814	7.135382	0.14779	200	0.959482	3.29954
	30.4243	2.93566	6.563512	0.22446	210	0.636247	7.43340
CDY-Y/CdSe	15.0531	5.88079	10.18453	0.18517	100	0.755302	5.31491
	25.9296	3.43343	6.866000	0.20958	102	0.678891	6.58984
	30.5959	2.91958	5.838438	0.14800	200	0.971276	3.21992
	36.2228	2.47792	5.540103	0.22584	210	0.645961	7.21157

3.3: Electrical properties

The resistivity, conductivity, and thickness values of undoped and Y-doped CdSe (with varying dopant concentration) are in table 3 and figure 4 illustrates the link between resistivity, conductivity and thickness of the films. The result shows that the Yttrium on CdSe films greatly affects the electrical properties and the film thickness. As the Yttrium molarity in CdSe increases from 0 to 0.04 mol%, the resistivity decreases from 6.210×10^{-6} Ω.m to a minimum value of 6.124×10^{-6} Ω.m with decreasing thickness of 150.21 nm to 136.13 nm and increasing conductivity values of 1.610×10^{5} $(\Omega m)^{-1}$ to 1.632×10^{5} $(\Omega m)^{-1}$. This result corresponds to that of Choudhary and Chauhan 2017, for swift heavy ion effect on electrodeposited CdSe and Pathak *et al.,* for CdSe:Sm grew via CBD technique [15], [24].

Table 3: Electrical parameters of CdSe and Y doped CdSe (at different dopant concentrations)

Label	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 0.01 mol%	145.32	6.192×10^{-6}	1.614×10^{5}
CDY 0.02 mol%	142.41	6.171×10^{-6}	1.620×10^{5}
CDY 0.03 mol%	138.21	6.150×10^{-6}	1.626×10^{5}
CDY 0.04 mol%	136.13	6.124×10^{-6}	1.632×10^{5}

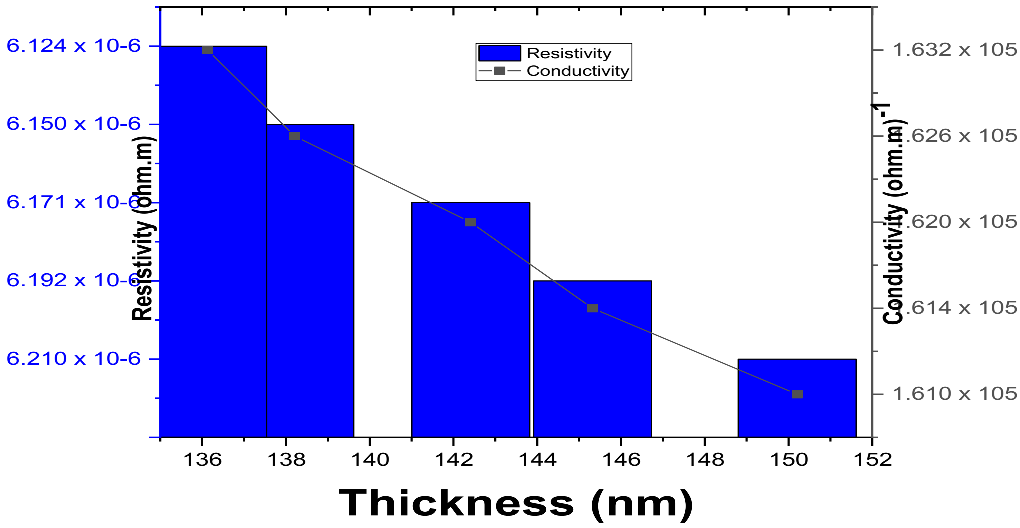

Fig. 4: A bar chart like a comparison of resistivity and conductivity of CdSe and YCdSe (for different dopant concentrations) with thickness.

3.4: Optical results

The optical results reveal that the incorporation of Y content into pure CdSe thin materials strongly influenced its optical features. Absorbance, transmittance and reflectance spectra of CdSe and Y-doped CdSe materials deposited from varying molarity of yttrium is displayed in fig. 5(a-c). The absorbance graph (fig. 5(a)) shows that the absorbance value of all the samples (both doped and undoped) decreases gradually as the incident wavelength increases. More so, the incoporation of yttrium as a dopant was discovered to have a significant impact on the absorbance value of undoped CdSe thin material. The absorbance value was seen to rise from 0.3 for undoped CdSe to as high as 1.3 for Y-CdSe at 0.03 mol% at a wavelength of 300 nm.

The transmittance spectra depicted in fig. 5(b) was a reverse of the absorbance spectra. The plot shows that the transmittance value of all the samples (both doped and undoped) increased gradually as the incident wavelength increases from 300 -1100 nm. The addition of yttrium to CdSe was observed to reduce its transmittance ability. For undoped, the maximum transmittance value was found to be 70% compared to Y-doped which is from 30% to 8% at the incident wavelength range of 800 nm to 1100 nm. The downturn in the transmittance value of YCdSe materials can be due to the improvement in the grain boundaries which was attained during doping [26].

The reflectance graph reveals that all the samples (both doped and undoped) had low reflectance. It was further observed that undoped CdSe thin material recorded its maximum reflectance of 0.2% at 300 nm which decreases as the wavelength increases while that of Y-doped films increases with an increase in wavelength with sample CDY (0.02 mol%) having the same maximum as the undoped at 1100 nm.

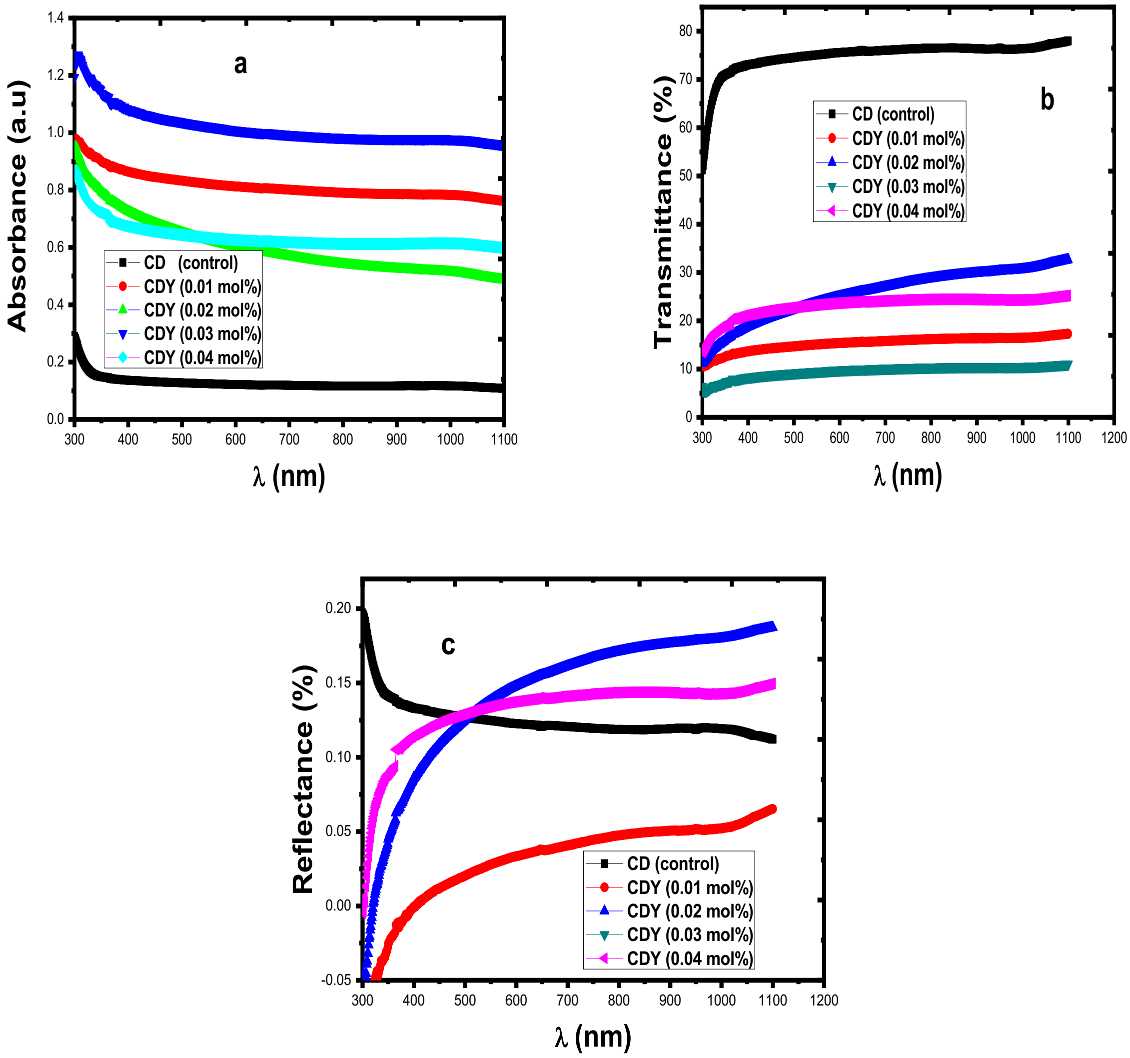

Fig. 5: Graph of (a) Absorbance (b) Transmittance and (c) Reflectance versus wavelength for CdSe and YCdSe at various dopant concentrations.

The energy bandgap for CdSe and YCdSe at different dopant concentrations (0.01 to 0.04 mol%) was deduced from the graph of $(\alpha h\nu)^2$ against hv as in figure 6. The energy bandgap for the samples was found to range from 1.41 to 1.71 eV which is in line with the literature [27]. From the plot, the bandgap energy was noticed to decrease from 1.71 eV for CdSe to 1.41 eV for doped as a result of the influence of the Y dopant on CdSe which acted as a substitutional impurity in its lattice location and also due to the creation of nanosized particles and there is no report on YCdSe before this study. Due to the narrowed energy bandgap exhibited by these doped samples, it will be a promising material for photovoltaic applications and solar cell fabrication in particular.

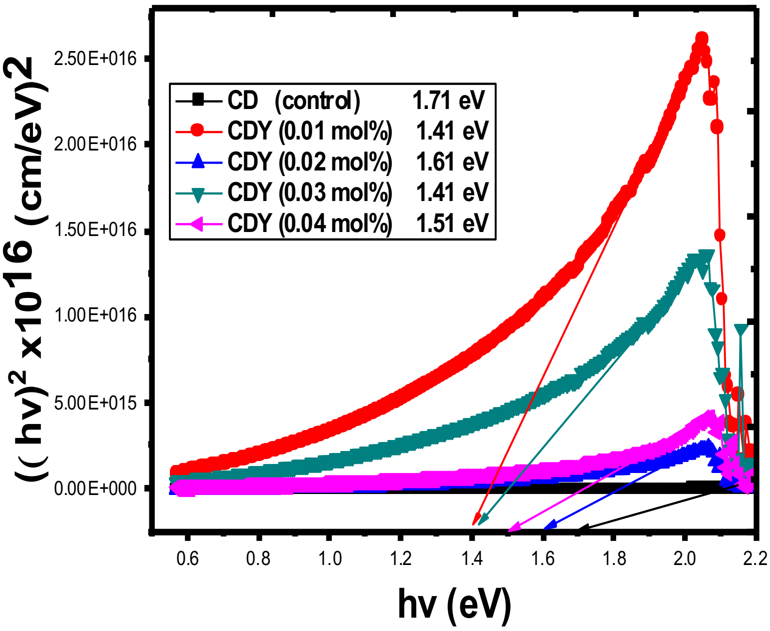

Fig. 6. Plots of $(\alpha h\nu)^2$ verse hν for CdSe and Y-doped CdSe at different dopant concentrations.

Figure 7 (a-c) show the plot of optical conductivity, extinction coefficient, and refractive index against hv for undoped CdSe and YCdSe at various dopant concentration. The extinction coefficient value decreases with an increase in photon energy for all the doped samples while the undoped CdSe remains almost constant throughout. More so, the addition of yttrium to pure CdSe increases its extinction coefficient. The sample doped with 0.01 mol% had the highest value when compared to others doped with 0.02, 0.03, and 0.04 mol% while the undoped CdSe had the lowest value. The high extinction coefficient value exhibited by the Y-doped CdSe makes it a very useful material for solar cell fabrication. From fig 7(b), the refractive index decreases with an increase in photon energy for all the Y-doped CdSe which shows normal dispersion behavior of the material but increases with an increase in photon for undoped CdSe. The addition of yttrium(Y) on pure CdSe increases its refractive index which decreases with an increase in s concentration of the Y-dopant. The CdSe sample with 0.01 mol% of yttrium and the undoped CdSe had the highest refractive index value of 2.6 at 0.6 eV and 2.1 eV respectively. For optical conductivity, all the samples exhibited a similar trend of almost a steady value with an increase in photon energy except for sample Y-doped CdSe (0.02 mol%) which increases with an increase in photon energy and also recorded the highest optical conductivity value amidst the other samples. It was also observed that the addition of Y dopant enhanced the optical conductivity of CdSe. The graph of real and imaginary dielectric constant verse hv for undoped CdSe and YCdSe at varying dopant concentrations are displayed in fig 8(a-b) respectively. In this study, the values of the real part are higher than those of the imaginary part. From the graph in fig 8(a), the real dielectric constant decreases with an increase in photon energy for all the Y-doped CdSe but increases with an increase in photon for undoped CdSe.

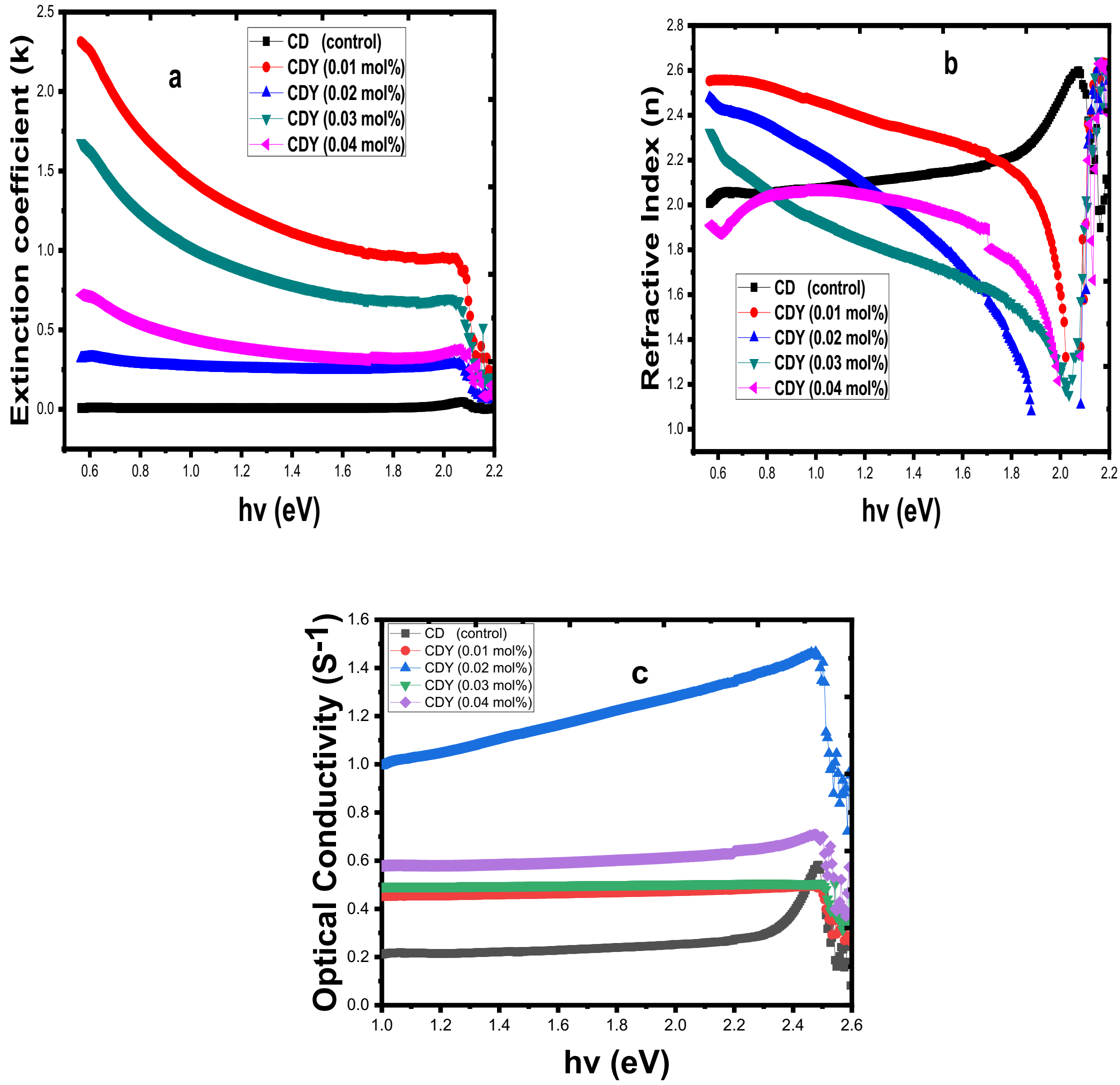

Fig. 7: Graph of (a) Extinction coefficient (b) Refractive index and (c) Optical conductivity against h*ν* for CdSe and YCdSe at various dopant concentrations.

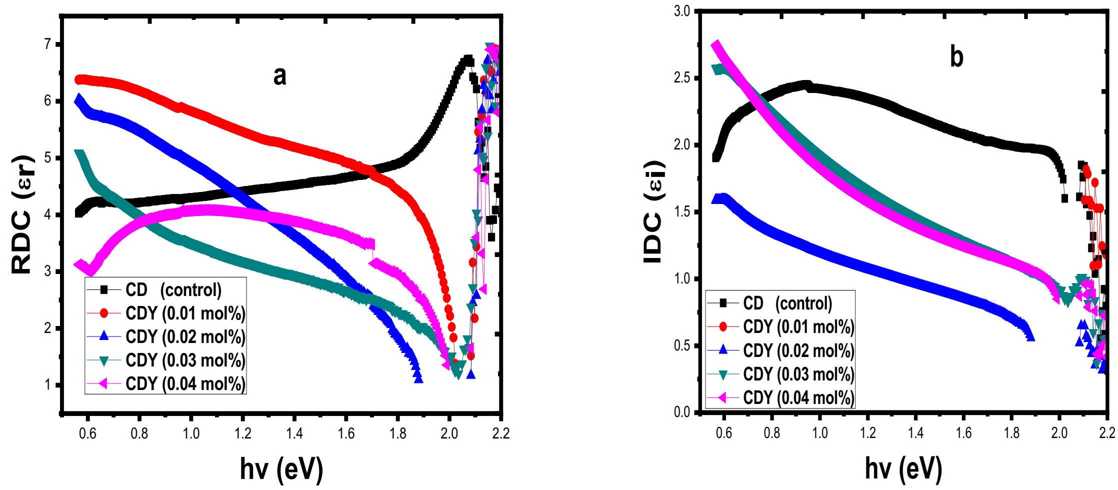

Fig. 8: Graph of (a) Real and (b) imaginary dielectric constant against h*ν* for CdSe and YCdSe at various dopant concentrations.

It was seen that the addition of 0.01 mol% of yttrium(Y) on pure CdSe increases its real dielectric constant value which decreases with further increase in the concentration of the Y-dopant. The imaginary dielectric constant of all the samples (both undoped and Y-doped CuSe) was seen to decrease with an increase in photon energy with CdSe doped with a higher concentration of yttrium (0.04 and 0.03 mol%) having the maximum

Conclusion

Using spray pyrolysis deposition technique undoped and Y-doped CdSe were grown on glass substrate at 400°C with Y concentration of 0.01, 0.02, 0.03, and 0.04 mol% accordingly. The as-deposited thin materials were characterized to ascertain the influence of Y dopant on the pure CdSe thin material. Elemental compositional analysis was carried out by EDX which confirmed the presence of the basic elements Cd, Se, and Y. The microstructure explored by use of SEM machine showed uniform films with dense surface morphology covering the whole substrate and without cracks. The addition of Y dopant was seen to utter the surface grain patterns. The structural results were obtained via XRD analysis. The XRD patterns revealed that the nature of all the synthesized thin materials is polycrystalline which possesses a hexagonal structure with the predilect orientation and highest intensity along the (100) plane. The incorporation of yttrium dopant was noticed to enhance the crystallinity of CdSe. The electrical studies carried out via a four-point probe showed that an increase in Y-concentration from 0 to 0.04m0l%, led to a decrease in the resistivity of CdSe with decreasing film thickness and increasing conductivity value. These electrical results confirm that the as-deposited thin materials as good semiconductors. Optical studies were carried out to record the absorbance of the undoped and Y-doped CdSe, other optical properties such as transmittance, reflectance, refractive index, energy band gap, optical conductivity, extinction coefficient, real and imaginary dielectric constants were obtained using appropriate mathematical relations. Energy band gap values deduced from $(\alpha h\nu)^2$ against ($h\nu$) graph showed energy band gap values ranging from 1.41 eV to 1.71 eV. Incorporation of Y dopant was seen to narrow the energy band gap of undoped CdSe from 1.71 eV t as low as 1.41 eV for CdSe doped with 0.01 and 0.03 mol% of Y. Optimization of CdSe thin materials properties via Y doping significantly improved its potential for use in photovoltaic applications and solar cell fabrication in particular.

Declarations

Funding: The authors received no funding for this research.
Conflicts of Interest: None to declare
Ethical Statement: The *paper* reflects the authors' *research* and analysis truthfully and completely.
Data Availability Statement: The data that support the findings of this study are available on request from the corresponding author

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