



# **Tuning structural, electrical, linear, and nonlinear optical properties of cadmium zinc telluride quantum dot thin flms**

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Quantum dots of Cd<sub>0.18</sub>Zn<sub>0.14</sub>Te<sub>0.68</sub> thin films of various thicknesses are deposited on a glass substrate **using inert gas condensation and characterized using many techniques. Structural analysis confrms the cubic polymorph of the thin flms. The particle size increased from 5.7 to 10.35 nm as the flm thickness increased from 10 to 100 nm. Bandgap calculations show two direct allowed transitions, one of which is 1.8 eV for diferent thicknesses. The other transition changes from the ultra-violet region (3.7 eV) for 10 nm thickness to yellow (2 eV) for 100 nm thickness, depending on the particle size. This result suggests that this material is suitable for use in multiple absorption layers of the same material rather than multilayers of diferent materials in tandem solar cells. The optical linear and nonlinear parameters highly depend on the particle size. Electrical conductivity shows intrinsic conduction with low activation energies from ambient temperature to 336 K.**

# **Introduction**

The use of dual semiconductor materials of zinc telluride and cadmium telluride thin flms is crucial in various signifcant scientifc and technological applications, such as solar cells and electronic devices  $[1-7]$  $[1-7]$ , light-emitting diodes  $[8]$  $[8]$ , and photode-tectors [\[9\]](#page-10-2). This significance is due to their electronic and optical properties, where the dual systems of CdTe and ZnTe have a wide direct bandgap that allows their application as absorbing layers in solar cells [\[10–](#page-10-3)[13](#page-10-4)], and they are also characterized by their high absorption coefficient that reaches  $10^5$  cm<sup>-1</sup> [[12–](#page-10-5)[15\]](#page-10-6).

To produce a signifcant change in the physical properties of these systems, a tripartite compound of cadmium zinc telluride (CdZnTe) must be achieved by either introducing zinc into CdTe or cadmium into ZnTe, resulting in diferent properties that make it a key component for various technological applications [[16](#page-10-7)[–19\]](#page-10-8). CdZnTe is considered one of the most signifcant chalcogenide materials and belongs to the II–VI ternary semiconductor compound. It is a promising candidate for several technological applications, such as in optoelectronics and tandem solar cells [\[20](#page-10-9)–[22](#page-10-10)], optoelectronics [\[23\]](#page-10-11), and radiation detectors [\[19](#page-10-8), [20](#page-10-9), [24](#page-10-12)[–26](#page-10-13)], as it is used as a photoanode for watersplitting applications [[27](#page-10-14)].

Until now, only a few researchers studied the nonlinear optical properties of CdZnTe using the Z-scan method; however, this study spectroscopically calculates both linear and nonlinear optical parameters and discusses them.

Consequently, the main objective of this study is to tune the optical and electrical properties of cadmium zinc telluride nanocrystalline thin films based on their particle size. The inert gas condensation technique was used in this study to grow nanocrystalline  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films and inspect their physical properties, including structural, morphological, electrical, linear, and nonlinear optical parameters based on the spectroscopic method.

#### **Results and discussion**

#### **Structural and morphological study**

Figure [1\(](#page-1-0)a) depicts the recorded EDX spectrum of the prepared cadmium zinc telluride thin flm of 100 nm thickness deposited



<span id="page-1-0"></span>**Figure 1:** (a) EDX spectrum of  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin film of 100 nm thickness, and (b–e) the difraction patterns of grazing incident in-plane X-ray (GIIXD) for  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  films of various thicknesses.



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on a glass substrate. The peaks of Cd, Zn, and Te are clarified in the spectrum, with atomic ratios are 18.25:13.82:67.93, respectively, as seen in the table inserted in Fig. [1\(](#page-1-0)a). Consequently, the obtained film stoichiometry can be written as  $Cd_{0.18}Zn_{0.14}Te_{0.68}$ . The excess of Te with 10 at% for antimony telluride material was previously reported by Cullis and Midgley [[28](#page-10-15)], and they discovered a congruence in X-ray difraction lines for the ICDD standard data and the sample with 10 at.% excess Te.

The phase analysis and internal crystal structure of  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films of various thicknesses (30–100 nm) deposited on a cleaned glass substrate were examined using the GIIXD technique. Figure  $1(b)$  $1(b)$ –(e) illustrates the X-ray diffraction patterns for all the synthesized films. These patterns confrmed that the flms were crystallized in a cubic structure and revealed difraction lines (111), (220), and (311) that are

consistent with the ICDD (Card No. 50-1439) of lattice parameter  $a = 6.343$  Å.

Notably, the lower flm thickness [30 nm seen in Fig. [1\(](#page-1-0)b)] has a GIIXD pattern with a very low intense difraction line at the (111) plane, resulting in inaccuracies in calculating its particle size. Therefore, it is predictable that the diffraction line of the plane (111) becomes extremely small or disappears in the case of the lowest flm thickness (10 nm). So, the crystallinity and structural nature will be examined from the electron diffraction patterns (EDPs) of HRTEM, which will discuss in the next part. In similar cases, the crystal structure of an extremely small flm thickness was studied using HRTEM difraction patterns, as studied by I. A. Mahdy et al. [\[29,](#page-10-16) [30](#page-10-17)] and M. A. Mahdy et al. [\[31](#page-11-0)]. Whereas, as the flm thickness is increased, the high



intensive peak becomes sharper, increasing the particle size, as calculated from Scherrer's equation [\[32](#page-11-1)]:

#### $D = k\lambda/\beta \cdot \cos(\theta)$ .

The particle size, *D*, determined from the most intensive line (111) has values of 8.6, 9.3, and 14.8 nm for flm thicknesses of 60, 80, and 100 nm, respectively. This result shows an improvement in the flm crystallinity as the flm thickness increases [\[33\]](#page-11-2).

Moreover, the structured nature and particle size of the synthesized  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  nanostructured thin films were inspected by HRTEM analysis. The HRTEM images shown in Fig. [2\(](#page-2-0)a) and (d) illustrate the particle distribution, shapes, and sizes of flm thicknesses of 10 and 30 nm. Similarly, the particles in Figs.  $2(g)$  and (j) and  $3(a)$  $3(a)$  show the micrograph images of film thicknesses of 60, 80, and 100 nm, respectively. All micrograph images in these fgures reveal nanoparticle distributions for the synthesized  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films. The estimated average particle size is 5.7, 7, 8, 9.1, and 10.35 nm for flm thicknesses of 10, 30, 60, 80, and 100 nm, respectively. Some previous reports have mentioned that the CdTe and ZnTe compounds' exciton Bohr radii are 7.3 nm [[34,](#page-11-3) [35\]](#page-11-4) and 4.6 nm [[36\]](#page-11-5), respectively. Whereas Lee et al. [[37](#page-11-6)] stated that the estimated Bohr radius of the  $Cd_{0.25}Zn_{0.75}Te$  compound is 6 nm. Compared with the X-ray and HRTEM results of our study, the particle radius (2.85–5.17 nm) of the prepared flms (10–100 nm in thickness) is smaller and nearly equal to the estimated Bohr radius [[37\]](#page-11-6). In other words, the prepared thin flms have strong quantum confinement, indicating their quantum dot (QD) formation. The



<span id="page-2-1"></span>**Figure 3:** (a–c) HRTEM images, and (d, e) micrograph images of FESEM of the  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  nanocrystalline thin films of 100 nm thickness.

EDPs for each flm thickness refect that all thin flms showed a crystalline phase, as depicted in Figs.  $2(c)$ ,  $(f)$ ,  $(i)$ , and  $(l)$  and  $3(c)$  $3(c)$ . The film's crystallinity was detected by EDP even at a thickness of 10 nm, and it appeared with low crystallinity (30 nm), as depicted in the GIIXD results. In addition, the crystallinity was illustrated in the magnifed lattice images for all flms that are situated between the orange dashed lines. The *d*-values of film



<span id="page-2-0"></span>**Figure 2:** HRTEM images of the Cd<sub>0.18</sub>Zn<sub>0.14</sub>Te<sub>0.68</sub> nanocrystalline thin films, (a–c) 10 nm, (d–f) 30 nm, (g–i) 60 nm, and (j–l) 80 nm.



thicknesses of 30–100 nm were illustrated on the attached lattice maps that are referred to by light blue arrows, as seen in Figs. [2](#page-2-0) and [3.](#page-2-1) The *d*-value for 10 nm thickness is written on the lattice image, as illustrated in Fig. [2\(](#page-2-0)b). The assigned *d*-values were 2.2, 3.66, 2.25, 3.6, and 3.67 Å for flm thicknesses of 10, 30, 60, 80, and 100 nm, respectively as depicted in Figs.  $2(b)$ ,  $(e)$ ,  $(h)$ ,  $(k)$ and  $3(b)$  $3(b)$ . The assigned *d*-values correspond to planes of (111) and (220) of  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  cubic structure, which is consistent with reference ICDD Card No. 50-1439 [\[38](#page-11-7)] as confrmed by the X-ray result.

The field emission scanning electron microscope (FESEM) images of a thin flm of 100 nm thickness as a representative sample were used to identify the surface morphology, as shown in Fig.  $3(d)$  $3(d)$  and (e). The micrographs of two magnification scales (2 μm and 500 nm) show good flm continuity with a regular grain distribution with very clear boundaries. The grains have a small average size ranging from 17 to 44 nm. These small grains ratifed the formation of nanostructured thin flms of the chalcogenide semiconductor compound,  $Cd_{0.18}Zn_{0.14}Te_{0.68}$ .

## **Optical studies**

Figure [4](#page-3-0)(a) and (b) depicts the recorded optical transmission, *T*, absorption, *A*, and refection, *R*, spectra for the investigated nanocrystalline thin films of different thicknesses. The values of *T* were inversely proportional to the flm thickness, whereby they decreased as the flm thickness increased due to the trapping of the incident light in the thicker flm than in the thinner one [Fig. [4\(](#page-3-0)a)]. Conversely, the condensed layers of the thicker flm increase the *R* values than those for a thinner flm [Fig.  $4(b)$ ]. The inset panel in Fig.  $4(a)$  represents the absorption spectra of the investigated nanocrystalline flms that clarify the shif of the absorption edge toward the higher wavelength as the film thickness increase. These absorption edge shifts reflect the decrease in the thicker flm's optical gap value [\[33](#page-11-2)]. Moreover, we discovered two steps in the absorption edges for the investigated flms in the *A* and *T* spectra, except for the flm of 100 nm thickness, which has only a single absorption edge, as seen in Fig. [4](#page-3-0)(a). All absorption edges were observed in the ultraviolet (UV) and visible wavelength spectral range.

The optical bandgap of the investigated thin films was calculated using the following formula [\[39,](#page-11-8) [40\]](#page-11-9);

$$
\alpha E = \beta (E - E_{\rm g})^p,
$$

where  $\alpha$  denotes the absorption coefficient that depends on the transmission and reflection values  $[40]$  $[40]$ ,  $E_g$  is the optical gap energy, *E* signifes an incident photon energy, *β* represents the bandwidth parameter and *p* denotes the power factor of transition mode. The  $E_{\rm g}$  calculations verified that the best linear fit refers to the direct allowed transition, i.e., the exponent *r* equal 1/2.



<span id="page-3-0"></span>**Figure 4:** Panel (a) and its inset show the transmission (*T*) and absorption (*A*) spectra, respectively, panel (b) shows the refection (*R*) spectra, and panels (c–g) represent the graph of (*αE*)<sup>2</sup> versus photon energy *E* for Cd<sub>0.18</sub>Zn<sub>0.14</sub>Te<sub>0.68</sub> nanocrystalline films of different thicknesses, denoting the first optical gap,  $E_{a1}$ , transition.





**NBLE**1: Obtained values of two transitions of the optical gap (E<sub>g3)</sub> dispersion energies (E<sub>g3),</sub> oscillator strength, F, both static dielectric constant (ε<sub>ξ</sub>) and refractive index (n<sub>3</sub>), ratio of carrier concen-

tration to effective mass ( $\frac{N}{\cos}$  ) and lattice dielectric constant ( $\varepsilon$ <sub>1</sub>), and the of CdZnTe nanocrystalline thin films

**IABLE 1:** Obtained values of two transitions of the optical gap (E<sub>ga)</sub>, dispersion energies (E<sub>osc</sub> and E<sub>dis</sub>), oscillator strength, F, both static dielectric constant (ε) and refractive index (n<sub>3</sub>), ratio of carrier

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The relations between  $(\alpha E)^2$  versus photon energy for the synthesized thin films are shown in Figs.  $4(c-g)$  $4(c-g)$  and  $5(a-d)$  $5(a-d)$ , revealing two transitions of optical gaps  $E_{\text{g}1}$  and  $E_{\text{g}2}$ . The transmission spectra [Fig. [4\(](#page-3-0)a)] and its inset panel of absorption spectra show two distinguishable linear portions for all flms, except for the higher flm thickness (100 nm), which has only one absorption edge. The two linear portions demonstrate the probability of the simultaneous occurrence of two separate pro cesses of optical transition described by the two optical gaps. The existence of two optical transitions was attributed to the spin–orbit splitting phenomena [[41\]](#page-11-10). Indeed, the two optical gap transitions were reported earlier for chalcogenide thin flms of CdSe, CdTe, and  $Bi_2S_3$  [[41](#page-11-10)[–43\]](#page-11-11). The values of the first optical gap,  $E_{\text{gl}}$ , transition were decreased from the UV absorption (UVA) region (3.7 eV) to the yellow region (2 eV) by increas ing the flm thickness from 10 to 100 nm, as shown in Fig. [4](#page-3-0) and Table [1](#page-4-0). However, the value of the second optical gap,  $E_{g2}$ , transition (1.8 eV) falls in the red spectral region for flms of 10-80 nm thickness, as revealed in Fig. [5](#page-5-0). This means that the evaluated optical bandgap values fall in the UVA, violet, blue, green, yellow, and red spectral regions. These results indicate that this substance can be used as a multilayer absorption mate rial rather than using layers of diferent substances in tandem solar cells.

The complex refractive index  $(n^* = n + ik)$  is used to describe an important optical property of various materials. From the real  $(n = (1 + \sqrt{R})/(1 - \sqrt{R}))$  and imaginary  $(k = \alpha \lambda/4\pi)$  parts of *n*\*, the optical parameters, such as dispersion and dissipation percentage, of the electromagnetic waves can be determined. Depending on the recorded refection spectra and calculated absorption coefficient, the refractive index, *n*, and the extinction coefficient (absorption index),  $k$ , were calculated for the investigated flms. Figure [5\(](#page-5-0)e, f) depicts the dependence of the calculated *n* and *k* values on the flm thickness, respectively. This result is consistent with the earlier recorded studies  $[33, 3]$  $[33, 3]$  $[33, 3]$ [42](#page-11-12), [44,](#page-11-13) [45\]](#page-11-14) for various semiconductor thin flms. Notably, in higher wavelength region (>900 nm), the refractive index value increase as the film thickness increases [Fig.  $5(e)$  $5(e)$ ] due to a denser arrangement of atoms, indicating crystallinity improvement.

The refractive index,  $n$ , is a key factor for obtaining both linear  $(X^L)$  and third-order nonlinear optical susceptibility  $(X^{NL})$ according to the following expressions [[46,](#page-11-15) [47](#page-11-16)]:

$$
X^{\mathcal{L}} = (n^2 - 1)/4\pi,
$$

$$
X^{\mathcal{NL}} = B(X^{\mathcal{L}})^4,
$$

<span id="page-4-0"></span>where *B* denotes a constant  $(1.7 \times 10^{-10} \text{ e.s.u.})$  and it is almost equal for all materials. The variant of  $X^{\text{L}}$  and  $X^{\text{NL}}$  with photon energy, E, for nanocrystalline  $\mathrm{Cd}_{0.18}\mathrm{Zn}_{0.14}\mathrm{Te}_{0.68}$  thin films with diferent thicknesses is clarifed in Fig. [6.](#page-5-1) From these fgures, the  $X^{\rm L}$  and  $X^{\text{NL}} = (n^2 - 1)/4\pi$ ,<br>  $X^{\text{NL}} = B(X^{\text{L}})^4$ ,<br>
3 denotes a constant  $(1.7 \times 10^{-10} \text{ e.s.u.})$  and it is almost<br>
or all materials. The variant of  $X^{\text{L}}$  and  $X^{\text{NL}}$  with photon<br> *E*, for nanocrystalline  $Cd_{0.18}Zn_{0.14}$ 



<span id="page-5-0"></span>**Figure 5:** (a–d) The graph of (αE)<sup>2</sup> versus photon energy *E*; denoting the second transition of optical gap, *E*<sub>q2</sub>, and (e, f) representative of refractive index, *n*, and absorption index, *k*, for nanocrystalline Cd<sub>0.18</sub>Zn<sub>0.14</sub>Te<sub>0.68</sub> thin films of different thicknesses.



<span id="page-5-1"></span>**Figure 6:** (a) Plot of linear susceptibility,  $X^L$ , versus photon energy, *E*, and (b–e) plot of the nonlinear susceptibility,  $X^{NL}$ , versus photon energy, *E*, for nanocrystalline  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films.



<span id="page-6-0"></span>**Figure 7:** (a) A plot of the inverse of  $(n^2 - 1)^{-1}$  versus  $E^2$ , (b) representative of  $n^2$  as a function of  $\lambda^2$ , and (c, d) a plot of nonlinear refractive index vs. wavelength for nanocrystalline  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films.

and nonlinear susceptibility is increased with flm thickness due to the increased carrier concentration. The increase in carrier concentration with flm thickness was previously reported [\[48](#page-11-17), [49](#page-11-18)].

For wavelengths>1000 nm [Fig. [5](#page-5-0)(e)], the *n* values gradually decrease with increasing wavelength, particularly for higher flm thicknesses of 60–100 nm, and are nearly constant for lower thicknesses of 10 and 30 nm. Blow the absorption edge, the *n* data can be examined using Wemple and DiDiomenico's concept of normal dispersion [\[50](#page-11-19)]:

$$
n^2 - 1 = E_{\text{dis}} E_{\text{osc}} / (E_{\text{osc}}^2 - E^2),
$$

where  $E_{osc}$  is the single oscillator energy and  $E_{dis}$  denote the dis-persion energy. Figure [7\(](#page-6-0)a) shows the relation between  $(n^2-1)^{-1}$ and the square value of the photon energy,  $E^2$ . The values of  $E_{\rm osc}$ and  $E_{dis}$  are obtained from the intercept with the  $(n^2-1)^{-1}$  axis and the slope of Fig.  $7(a)$  $7(a)$ , respectively. The obtained values of both oscillator and dispersion energies of the investigated thin flms are recorded in Table [1](#page-4-0).

Subsequently, important optical parameters that depend on  $E_{\rm osc}$  and  $E_{\rm dis}$  values can be calculated. These important parameters are the static refractive index ( $n_s = \sqrt{1 + E_{dis}/E_{osc}}$ ) [\[51](#page-11-20)–[53](#page-11-21)], oscillator strength  $(F = E_{osc}E_{dis})$ , and both moments  $(M_{-1})$  and  $(M_{-3})$ , which refers to the interband transition strength. The two moments are expressed from relations [\[53\]](#page-11-21):

$$
E_{\text{osc}}^2 = \frac{M_{-1}}{M_{-3}}
$$
 and  $E_{\text{dis}}^2 = \frac{M_{-1}^3}{M_{-3}}$ .

The static dielectric constant ( $\varepsilon_s = n_s^2$ ) can be determined when the  $n_s$  is calculated. Table [1](#page-4-0) lists the calculated values of  $n_s$ ,  $\varepsilon_s$ , *F*,  $M_{-1}$ , and  $M_{-3}$  and their values generally increase as the film thickness increases. This result indicates that the increase in flm thickness causes crystallization improvement due to denser films. Moreover, the ratio of carrier concentration/effective mass



 $\left(\frac{N}{m^*}\right)$  and lattice dielectric constant  $(\varepsilon_L)$  can be estimated at a higher wavelength from the following relation [\[54,](#page-11-22) [55\]](#page-11-23):

$$
n^2 = \varepsilon_{\rm L} - \left(\frac{e^2 N}{\pi c^2 m^*}\right) \lambda^2,
$$

where *e* and *c* symbolize the charge of electron and light velocity, respectively. The plot of  $n^2$  versus  $\lambda^2$  is illustrated in Fig. [7](#page-6-0)(b), and from its slope and linear extrapolation intercept at  $\lambda = 0$ , the values of  $\left(\frac{N}{m^*}\right)$  and  $\left(\varepsilon_{\text{L}}\right)$  can be assigned, respectively, and recorded in Table [1](#page-4-0). The values of  $\varepsilon_{\text{L}}$  are noticeably large compared with those of  $\varepsilon_s$  for the investigated films (Table [1](#page-4-0)). This result refects the free carrier role in the polarization process inside the flms, which is due to the flm's exposure to electromagnetic wavelength.

Further, below the optical gap (i.e., absorption edge) region, the nonlinear refractive index  $(n_2)$  can be evaluated according to the following formula [[46,](#page-11-15) [56](#page-11-24)]:

$$
n_2 = 12\pi X^{\rm NL}/n_s.
$$

Figure  $7(c, d)$  $7(c, d)$  depicts the calculated nonlinear refractive index,  $n_2$ , as a function of wavelength. The  $n_2$  behavior showed a rapid decrease in the lower wavelength region, which tends to be constant at a higher wavelength for the flms under study. In addition, the values of  $n_2$  are contingent on the thickness of the flm.

Some valuable parameters can be computed from the optical data, for example, interband transition strength  $(J_{CV})$  and surface/volume energy loss functions ( $V_{\text{ELE}}$  and  $S_{\text{ELE}}$ ).

The two parts of the dielectric constant, real ( $\varepsilon_r = n^2 - k^2$ ) and imaginary ( $\varepsilon$ <sub>i</sub> = 2*nk*), are considered key parameters in determining some signifcant optical parameters, such as interband transition strength and two-loss functions (surface and volume energy loss)*.*

The material's electronic structure provides information about the density of states for the valence and conduction bands, as well as the electronic transitions from occupied to unoccupied bands [\[57](#page-11-25)]. These electronic or interband transitions revealed the optical response in terms of the complex interband transition strength, which is linked to the dielectric constant, as expressed in the following formula [[57](#page-11-25), [58](#page-11-26)]:

$$
J_{\rm CV} = J_{\rm CV1} + J_{\rm CV2} = \frac{m_{\rm e}^2}{e^2 \hbar^2} \frac{E^2}{8\pi^2} (\varepsilon_{\rm i} + i\varepsilon_{\rm r}),
$$

where  $J_{\text{CV1}}$  and  $J_{\text{CV2}}$  implies the real and imaginary parts of the complex  $J_{CV}$ , whereas *e* and  $m_e$  represent the electron charge and mass, respectively.

Figure  $8(a, b)$  shows the interband transitions versus photon energy for nanocrystalline  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films. The real part of the interband transition strength increases with the flm thickness up to around  $4 \text{ eV}$  [Fig.  $8(a)$  $8(a)$ ], whereas the imaginary part increases in low energy up to about 1.5 eV, then it takes an irregular behavior with thickness in the higher energy values



<span id="page-7-0"></span>**Figure 8:** (a, b) Variation of real ( $J_{CV1}$ ) and imaginary ( $J_{CV2}$ ) parts of interband transition strength with energy, and (c–g) plot of surface and volume energy loss functions (S<sub>ELF</sub> and  $V_{\text{ELF}}$ ) vs. energy (*E*) for Cd<sub>0.18</sub>Zn<sub>0.14</sub>Te<sub>0.68</sub> thin films.



[Fig. [8\(](#page-7-0)b)]*.* Higher flm thicknesses have a higher absorption value, which causes the real and imaginary components of  $J_{CV}$ to increase more than lower flm thicknesses. Normally, photon energy increases,  $J_{CV}$  values increase, indicating that the possibility of materials' electronic transition increases with energy.

In addition, the real part of  $J_{CV}$  gives a significant optical response to photon energy at around 1.5 eV, whereas the imaginary part has a response at about 0.7 eV. This result provides strong evidence for the photon absorption increases in the synthesized thin flms afer around 1.5 and 0.7 eV for the real and imaginary parts of  $J_{CV}$ , respectively. The photon absorption results in electronic excitation and causes electron transport from the valence band to the conduction band [\[58\]](#page-11-26)*.*

The movement of electrons inside the materials is responsible for energy loss, and both functions of volume and surface energy loss were used to determine the probability of losing energy. The two terms  $V_{\text{ELF}}$  and  $S_{\text{ELF}}$  depend on the oscillation dielectric functions, εr and εi*,* as expressed in the following formulas [[59](#page-12-0), [60](#page-12-1)]:

$$
V_{\text{ELF}} = \frac{\varepsilon_{\text{i}}}{\varepsilon_{\text{r}}^2 + \varepsilon_{\text{i}}^2},
$$

$$
S_{\text{ELF}} = \frac{\varepsilon_{\text{i}}}{(\varepsilon_{\text{r}} + 1)^2 + \varepsilon_{\text{i}}^2}.
$$

Figure [8\(](#page-7-0)c–g) depicts the computed  $V_{\text{ELF}}$  and  $S_{\text{ELF}}$  of the synthesized nanostructured thin films. The two-loss functions revealed the same behavior for each thickness, and it was observed that  $V_{\text{ELF}}$  had larger values than  $S_{\text{ELF}}$  for all films. Both functions increased with a photon energy range of around 1.5–4 eV for the two thicknesses of 10 and 30 nm and from around 1.5–3.3 eV for a 60 nm thickness. However, there are increments from around 1.5–2.3 eV for a thickness of 80 nm and around 1.5–2 eV for a thickness of 100 nm.

The difference in the values of both  $V_{\text{ELF}}$  and  $S_{\text{ELF}}$  loss functions may be attributed to the electronic transitions. In other words, the free carriers that traverse through the interior difer from those transferred through the surface because of the flm thickness.

Notably, the aforementioned optical results showed that introducing the Zn element into CdTe to attain the CdZnTe materials signifcantly changes the optical bandgap of their thin flms compared with previous studies [[31](#page-11-0)]*.*

#### **Temperature dependence of DC electrical conductivity**

Figure [9](#page-8-0) depicts the DC electrical conductivity of the asdeposited nanostructured flms, which reveals a normal semiconductor behavior. The conductivity slowly increases as the temperature increases from room temperature (300 K) up to around 330 K, and then starts to take a higher rate of increment to 473 K. The electrical conductivity values decrease as the



<span id="page-8-0"></span>**Figure 9:** Electrical conductivity as a function of (1000/*T*) of the thin flms of diferent thicknesses of 10–100 nm.

flm thickness increases, indicating the growth of particle size (Table [1\)](#page-4-0). In this case, the enhancement in electrical conductivity is attributed to the formation of nanosized particles accord-ing to the core–shell model [[61](#page-12-2)]. This result was also confirmed by the previous report of El Zawawi and Mahdy [\[62\]](#page-12-3) for another nanostructured thin film stoichiometry  $(Cd_{0.23}Zn_{0.77}Te)$ .

The activation energy was evaluated during the heating process using Mott's equation [\[63](#page-12-4), [64\]](#page-12-5):

$$
\sigma(T) = \sigma_0 \cdot \exp\left(-\frac{W_{dc}}{KT}\right),\,
$$

where  $W_{dc}$  is the activation energy,  $K$  denotes Boltzmann's constant, and *T* is the measured absolute temperature.

At the low-temperature range from room temperature " $T_{Room}$ " to around 336 K, it was observed that the activation energy ( $W_{dc}$ ) due to extrinsic conduction of impurity carriers increases from 0.036 to 0.17 eV as the flm thickness increases from 10 to 80 nm, respectively. However, its value decreases again to 0.059 eV for higher film thickness (100 nm). The activation energy represents around 1.44, 5.12, 6.92, and 6.8 of the *KT* value, which increases as the flm thickness increases from 10 to 80 nm and around 2.35 *KT* for 100 nm. However, in hightemperature regions "conductivity strong-dependent on temperature" the activation energy is attributed to the intrinsic conduction due to the intrinsic carriers since the activation energy values are close to half of the ionization energies of impurity carriers [[65\]](#page-12-6)*.*

## **Conclusion**

Nanocrystals of the ternary chalcogenide semiconductor system of  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  thin films were successfully prepared in the form of quantum dots. Their electrical, structural, morphological, linear, and nonlinear optical properties were



investigated in detail. A cubic structure was identified for nanocrystalline thin flms via structural investigation. Strong confnement was achieved in the flms, as proved by the morphological study and particle size determination. The optical bandgap is successfully tuned by particle size controlled by the flm thickness; the particle size increases from 5.7 to 10.35 nm as the film thickness increases from 10 to 100 nm. There were two optical transitions of the flms, one reduced from 3.7 eV at 10 nm flm thickness to reach 2 eV at 100 nm, including the absorption of diferent colors for each thickness, whereas the other transition has a fxed value of 1.8 eV that falls in the red region. These variations in the optical bandgap from 3.7 to 1.8 eV cover the UVA and visible spectral light regions. Consequently, the prepared thin flms are considered a candidate for multilayer solar cells made of the same material but with layers of varying thicknesses. The determination of linear and nonlinear optical parameters is signifcantly infuenced by the flm thickness (i.e., particle size).

# **Experimental**

Five thicknesses of  $Cd_{0.18}Zn_{0.14}Te_{0.68}$  were deposited on a glass substrate after undergoing the necessary cleaning process. The deposition process was carried out using the inert gas condensation technique [[66\]](#page-12-7). All deposited flms of 10, 30, 60, 80, and 100 nm thickness were inspected using different techniques. The grazing incident in-plane X-ray difraction (GIIXD, Empyrean Panalytical instrument—Netherlands) was used to determine the phase purity. The shape and particle size were determined using a high-resolution transmission electron microscope (HRTEM) Joel-1230, Japan. A FESEM (Quanta FEG 250, Czech Republic) was used to study the surface morphology and energy dispersive X-ray (EDX) analysis for composition determination of the highest flm thickness. Optical measurements were collected at ambient temperature using a spectrophotometer [JASCO V-570, Japan]. The electrical conductivity was measured during isochronal heating from room temperature up to 473 K in an evacuated system (0.1 mbar).

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# **Author contributions**

IAM: Resources, Conceptualization, Investigation, Analysis, Writing, Review, Editing, and Project Administration. SAM: Formal Analysis. MAM: Resources, Conceptualization, Investigation, Analysis, Writing Original Draf, Review, and Editing.

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# **Data availability**

The datasets generated during and/or analyzed during the current study are available on request from the corresponding author.

# **Declarations**

**Conflict of interest** The authors declare that they have no known competing fnancial interests or personal relationships that could have appeared to infuence the work reported in this paper.

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