

Growth, crystal structure and theoretical studies of energy and optical properties of $\text{CdTe}_{1-x}\text{Se}_x$ thin films

Kashuba A.I., Ilchuk H.A., Petrus R.Yu., Semkiv I.V., Zmiyovska E.O.

Lviv Polytechnic National University, Lviv, Ukraine



Contact information: Andrii Kashuba; AndriyKashuba07@gmail.com; https://www.researchgate.net/profile/Andrii_Kashuba

Table I

Structure parameters of $\text{CdTe}_{0.9}\text{Se}_{0.1}$ thin film.

Structure type	ZnS
Space group	$F-43m$
Unit-cell constants	$a = 6.395(3) \text{ \AA}$ $V = 261.6(4) \text{ \AA}^3$
D , nm	53.82
δ , nm^{-2}	$3.45 \cdot 10^{-4}$
ε	$8.1 \cdot 10^{-4}$
d , μm	~ 1.2

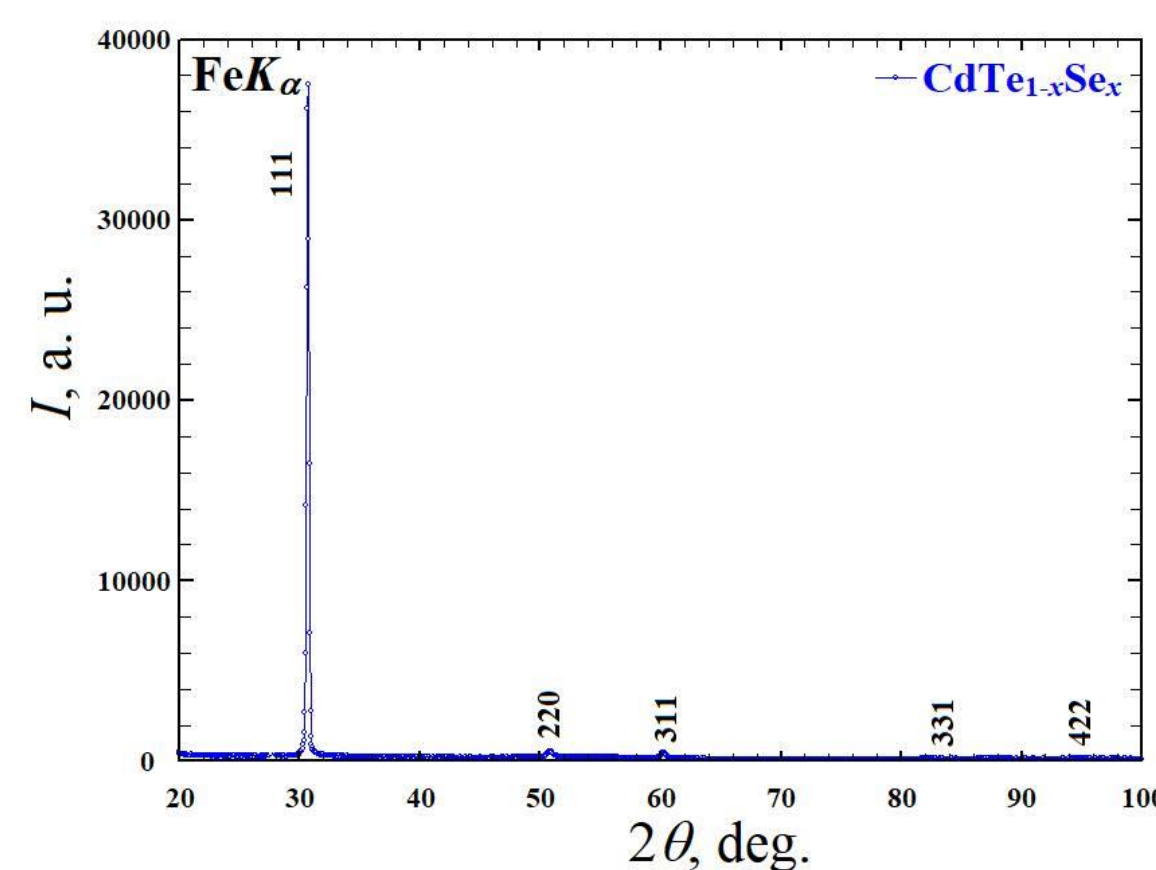


Fig. 1. XRD pattern of $\text{CdTe}_{0.9}\text{Se}_{0.1}$ thin film.

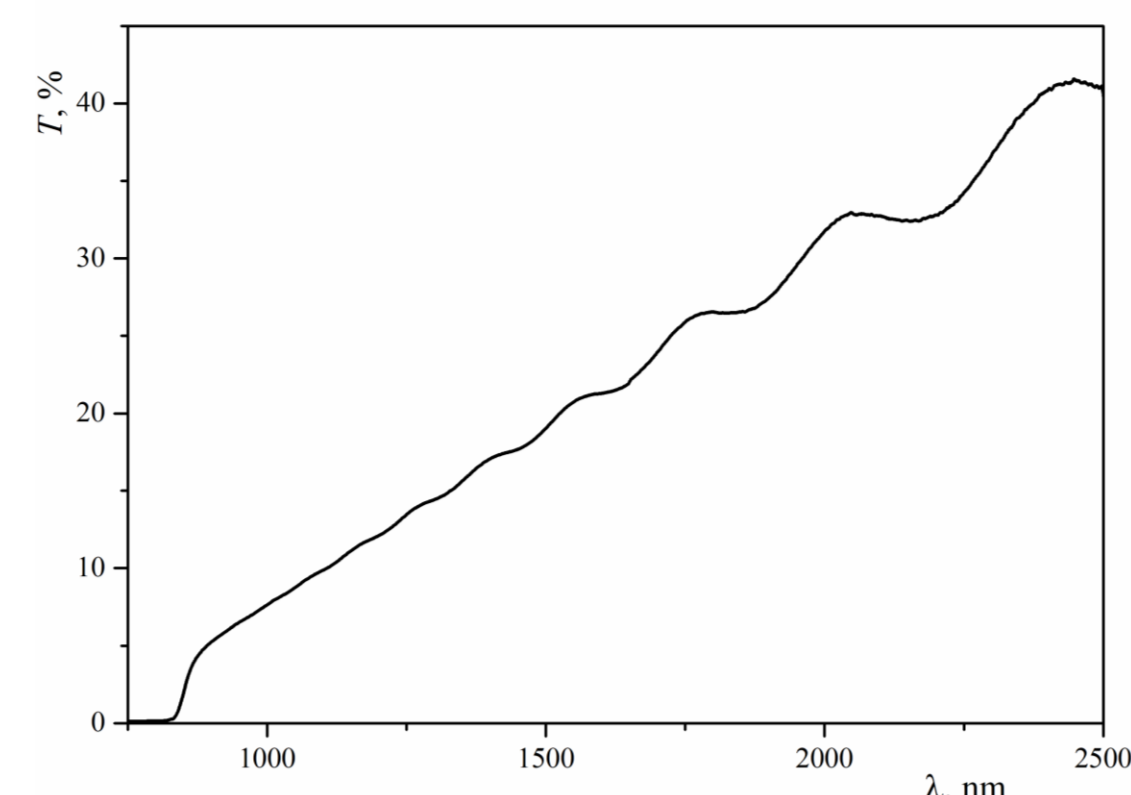


Fig. 3. Transmission spectra of $\text{CdTe}_{0.9}\text{Se}_{0.1}$ thin film.

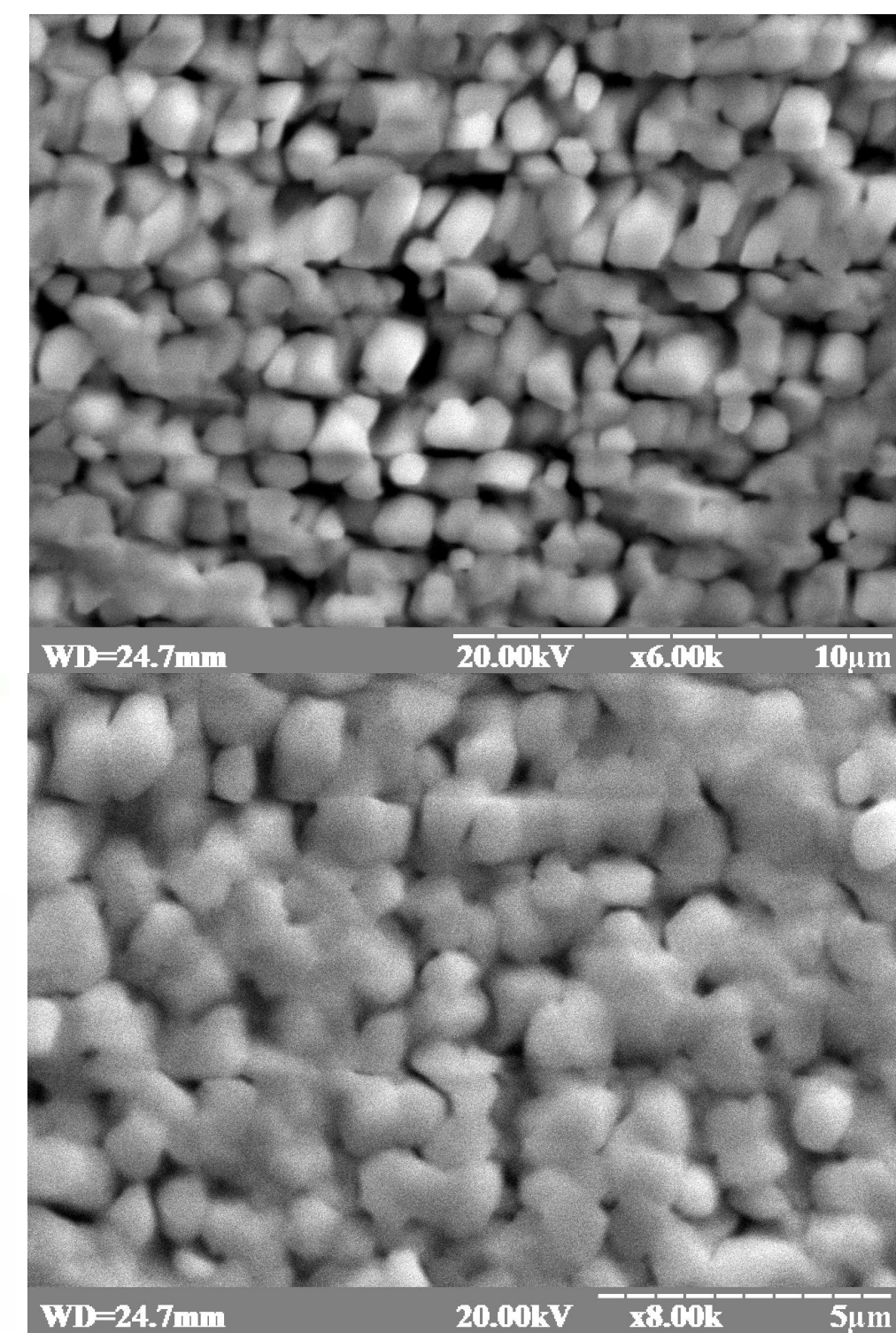


Fig. 2. Surface morphology of the $\text{CdTe}_{0.9}\text{Se}_{0.1}$ thin film.

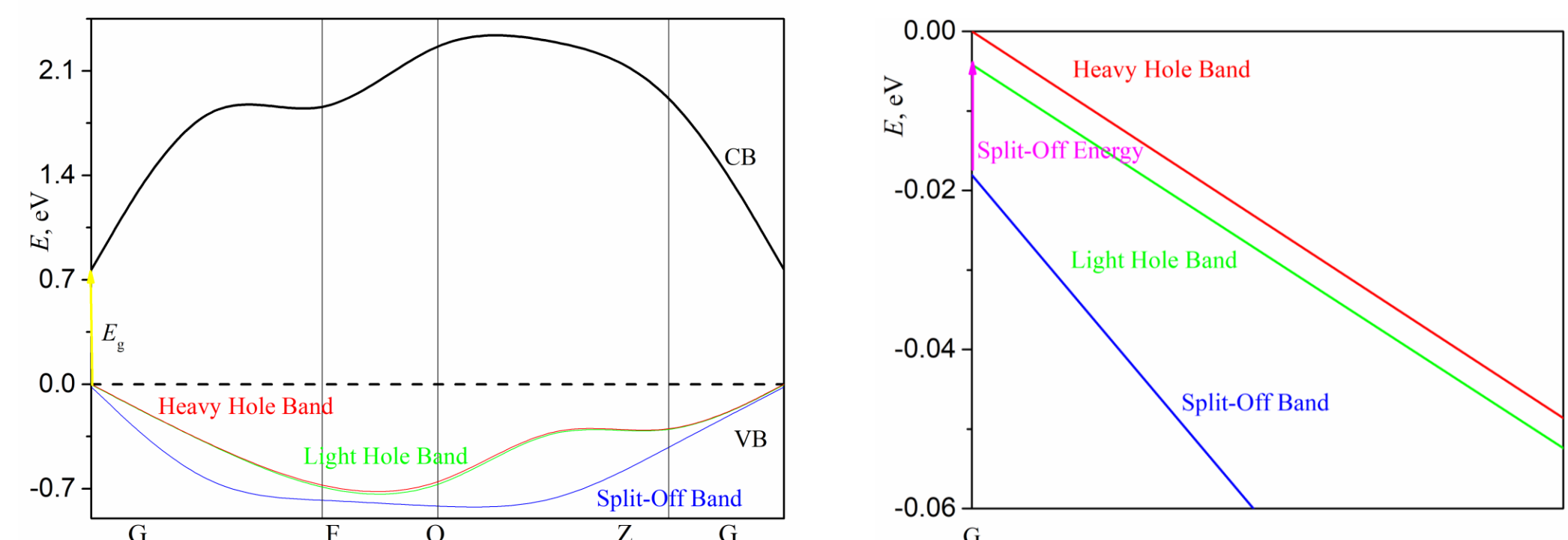


Fig. 4. Part of energy band diagram of $\text{Cd}_{16}\text{Te}_{15}\text{Se}$ solid state solution.

Introduction: The $\text{A}^{\text{II}}\text{B}^{\text{VI}}$ semiconductor compounds and their solid solutions, such as CdTeSe , have important applications such as infrared detectors, solar cells and other devices [1]. Despite the recent intensive experimental and theoretical study of these materials some of the fundamental parameters are currently unknown, primarily mechanical properties. This information is very important for modeling and building parts for optical and electronic devices.

The CdTeSe solid state solutions may be considered as a particular class of semiconductor materials having promising optical parameters for practical applications. This is due to the clear band gap E_g dependence on the tellurium content x of the material, $\text{CdTe}_{1-x}\text{Se}_x$ (CTS). The band gap changes from $E_g = 1.44 \text{ eV}$ for CdTe to $E_g = 1.68 \text{ eV}$ for CdSe [1]. It is important also that the above values of band gaps correspond to the near IR photon energy range, in which many commercial laser sources are accessible. The CdTe compounds have a cubic (zinc blende) structure [2], whereas CdSe compounds, depending on the growth conditions, may have both zinc blende and wurtzite (hexagonal) structures at normal conditions [3, 4]. According to the phase diagram [5] the crystallization of CTS is possible into cubic structure with selenium concentration $x \leq 0.33$ and into wurtzite one with corresponding concentration $x \geq 0.55$.

Methods: CTS thin film was prepared by quasi close-space sublimation method. The glass substrates were $\sim 14 \text{ mm}$ in diameter were used for deposition CTS thin films. Before the films deposition, the substrate surface was cleaned by boiling in a high purity CCl_4 solution during 0.5 h. The deposition of CTS films was conducted on a quartz substrate from polycrystalline $\text{CdTe}_{0.5}\text{Se}_{0.5}$ powder.

The phase analysis and crystal structure refinement was examined with using X-ray diffraction data. The thickness of the films was also measured on a Veeco profilometer (model Dektak 8). The surface morphology of the obtained CTS films was studied using the JSM 6700F scanning electron microscope (SEM-EDS). The spectral dependences of optical transmittance of the obtained samples were measured in the visible and near infrared regions (300-2500 nm) at room temperature using the spectrometer Shimadzu UV-3600.

The band structure and related properties of $\text{Cd}_{16}\text{Se}_{15}\text{Te}$ solid state solutions have been calculated in the framework of the density functional theory (DFT). In the present calculations, the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBESOL) exchange-and-correlation functional were utilized.

Results: CTS thin film crystallize in cubic structure (structure type –ZnS, space group $F-43m$, with unit-cell constants $a = 6.395(3) \text{ \AA}$ and $V = 261.6(4) \text{ \AA}^3$). No additional peaks (from X-ray analysis) belonging to other phases can be detected thereby indicating the formation of pure single ZnS phase (see Fig. 1). From X-ray analysis we obtained that $x \approx 0.1$.

The composition of the film was $x = 0.1$. Se content in this polycrystalline film was much lower than that found in the source (see experimental details). This composition-change is also observed when depositing $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ films, and is caused by the nonequilibrium deposition of the CSS growth process.

The crystallite size (D) was estimated from the peaks broadening using Sherrer's equation (1).

$$D = \frac{0.9 \cdot \lambda}{B \cdot \cos \theta} \quad (1)$$

where, λ is the wavelength of X-rays, B is fullwidth half maximum (FWHM) and θ is the Bragg's angle. The strain (ε) and the dislocation density (δ) were calculated using the following relations (2) and (3). The parameters obtained from X-ray diffraction are listed in table 1.

$$\delta = \frac{1}{D^2} \quad (2) \quad \varepsilon = \frac{\Delta(2\theta) \cdot \cos \theta}{4} \quad (3)$$

The surface morphology of the synthesized films is given in Fig. 2. The energy dispersive X-ray (EDX) study provides a way of analysis the chemical composition of materials.

Fig. 3 shows the transmission spectrum of the CTS films. There is a clear absorption edge near $\sim 805 \text{ nm}$ (close to CdTe at room-temperature 1.44 eV [2]).

The calculated part of the band energy structure of $\text{Cd}_{16}\text{Te}_{15}\text{Se}$ is presented in Fig. 4. Here, the Fermi level E_F corresponds to the energy $E = 0$. The band gap of $\text{Cd}_{16}\text{Te}_{15}\text{Se}$ is found to be of the direct type, $E_g^{(d)} = 0.767 \text{ eV}$ (Fig. 4).

References

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