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Full Length Research Paper

Studies on mass attenuation coefficients, effective atomic and electron numbers for $Cd_{1-x}Zn_xTe$ alloy at photon energies of 10 to 100 keV

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The physical parameters calculated using Full Potential Linear Muffin Tin Orbitales FP-LMTO method is satisfying. Using the photon mass attenuation coefficient obtained via XCOM data of $Cd_{1-x}Zn_xTe$ compound, the effective atomic number and the effective electron number were determined in the energy range of 10 to 100 keV. The effective atomic and electron numbers are linearly related and they also depend on the incoming photon energies and weight fractions of elements present in $Cd_{1-x}Zn_xTe$. This work aimed at the estimation of the Z_{eff} and the N_{eff} of $Cd_{1-x}Zn_xTe$ in the energy range of 10 to 100 keV. In the energy range of 40 to 100 keV, the effective atomic and electron numbers were found to be constant. The Z_{eff} and the N_{eff} decrease with the increase of the zinc concentration in the material. The effective atomic number takes values between the lowest Z = 30 of zinc and the highest Z = 52 of tellure in ZnTe and the ternary $Cd_{1-x}Zn_xTe$. But for CdTe, it takes values between Z = 42 of cadmium and Z = 52.

Key words: $Cd_{1-x}Zn_xTe$, XCOM Data, effective atomic number and effective electron number.

INTRODUCTION

The $Cd_{1-x}Zn_xTe$ alloy is a very important material for the manufacture of detectors, for this reason we need to calculate accurately the effective atomic and electron numbers. First, we have to calculate the mass attenuation coefficient (μ/ρ), which is a measure of the average number of interactions between incident photons and matter, that occur in a given mass-per-unit area thickness of the substance encountered (Woods, 1982). This coefficient can be usually calculated via XCOM data which is a computer program developed by (Berger and Hubbell, 1987) for different elements, mixtures and compounds between 1 keV to 100 GeV. In the ternary materials like $Cd_{1-x}Zn_xTe$, a single number can not represent the atomic number as in the case of an element. This number is defined as the "effective atomic number" (Z_{eff}) and it is a convenient parameter for evaluation of photon interaction with a medium (Hine, 1952). The effective electron number (N_{eff}) is another fundamental parameter describing the photon-matter interaction which is defined as the electron per unit mass of the absorber (Shivalinge et al., 2005). Several works have been carried out to determine the effective atomic and electron numbers for different materials (Hine, 1952; Kumar and Reddy, 1997; Guru et al., 1998; Murty et al., 2000; Shivaramu et al., 2001; Akkurt et al., 2005; Manohara and Hanagodimath, 2007a, b; Manohara et al., 2008; Ozdemir and Kurudirek, 2009; Demir and Han, 2009; Akkurt, 2009; Kurudirek et al., 2010; Bastug et al., 2010; Kirdsiri et al., 2011; Medhat, 2011; Han et al., 2012).

$Cd_{1-x}Zn_xTe$ crystals attract a lot of attention due to their characteristics which make them useful for a variety of applications that stretch from X-ray and gamma ray detectors (Zanio, 1978; Prias-Barragan et al., 2006) to optoelectronic devices such as far infrared detectors (P.W. Krusse et al, 1981; Yasuda et al., 2005). CdTe and CdZnTe detectors ensure high detection efficiency and good room temperature performance due to their physical properties, that is, the high atomic number (Z_{max} = 52), the

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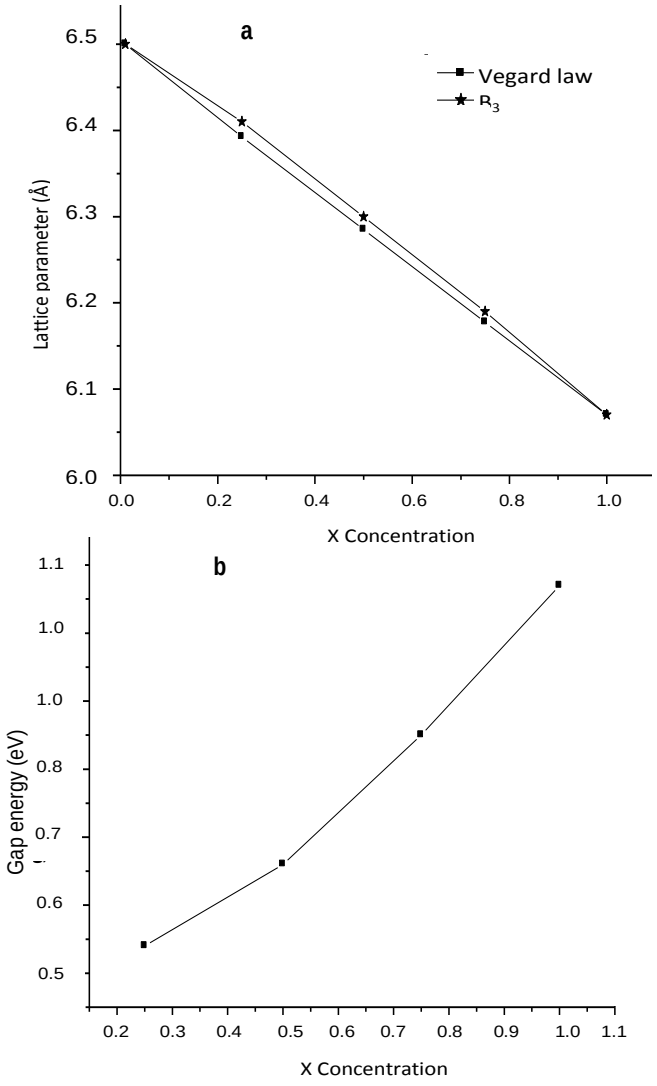

Figure 1. Variation of the lattice parameter **(a)** and the gap energy **(b)** with the concentration x of Zn in $Cd_{1-x}Zn_xTe$.

high density (CdTe: r = 6.20 g/cm^3; CdZnTe: r = 5.78 g/cm^3) and the wide band gap (CdTe: E_G~1.44 eV; CdZnTe: E_G~1.57 eV) (Abbene et al., 2010).

The aim of this work is to make an attempt to estimate theoretically effective atomic and electron numbers in the energy range between (10 to 100 keV) for $Cd_{1-x}Zn_xTe$ alloy. We have introduced the part of results and discussion with our abbreviate physical study of some important parameters of $Cd_{1-x}Zn_xTe$ using FP-LMTO method. In second, we have presented our results of calculations for Z_{eff} and N_{eff} using the XCOM computer program.

MATERIALS AND METHODS

For the characterization of $Cd_{1-x}Zn_xTe$, we have presented some physical properties which were performed within the first- principle Savrasov version of the full potential linear muffin-tin orbital (FP-LMTO). The exchange-correlation energy of electrons is described in the local density approximation (LDA) using the parameterization of Perdew and Wang, (1992).

In our study we use a ternary compound which is a mixture between Cd, Zn and Te, so the mass attenuation coefficient is calculated by (Jackson and Hawkes, 1981):

$$\frac{\mu}{\rho} = \sum_i \omega_i \left(\frac{\mu}{\rho}\right)_i \quad (1)$$

Where ω_i is the proportion by weight of the ith constituent element, $\left(\frac{\mu}{\rho}\right)_i$ is mass attenuation coefficient of constituent element.

The total atomic cross section (σ_t) can be obtained from the knowledge of theoretical values for the mass attenuation coefficients by the following relation (Wang et al, 1995):

$$\sigma_t = \frac{1}{N_a}\sum_i f_i N_i \left(\frac{\mu}{\rho}\right)_i \quad (2)$$

Where N is the atomic mass of $Cd_{1-x}Zn_xTe$ and N_A is the Avogadro's number. The total electronic cross section (σ_e) is given by (Singh et al, 2002):

$$\sigma_e = \frac{1}{N_a}\sum_i \frac{f_i N_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i \quad (3)$$

Where Z_i is the atomic number of the ith element in the compound. The total atomic cross section and the total electronic cross section are related to the effective atomic number Z_{eff} of a material consisting of different elements through the following relation (Singh et al., 2002):

$$Z_{eff} = \frac{\sigma_t}{\sigma_e} \quad (4)$$

Finally, the effective electron number (number of electrons per unit mass) can be calculated using the following expression:

$$N_{eff} = \frac{N_A}{N} Z_{eff} \sum n_i \quad (5)$$

RESULTS AND DISCUSSION

Physical properties

Figure (1a) has presented the variation of the lattice parameters depending on the concentration of the zinc in $Cd_{1-x}Zn_xTe$ with the Vegard's law. We have found that our calculations exhibit a good agreement with the latter with a small deviation of (-0.06875). From this figure, we have found that the lattice parameter is inversely proportional to the concentration of zinc and. The computed band structure of $Cd_{1-x}Zn_xTe$ using both LDA gave a direct band gap Γ- Γ for CdTe, $Cd_{0.75}Zn_{0.25}Te$, $Cd_{0.50}Zn_{0.50}Te$, $Cd_{0.25}Zn_{0.75}Te$ and ZnTe which are equal to 0.41, 0.54, 0.66, 0.85, 1.07 eV respectively. It is well known that LDA underestimates energy gaps. From Figure (1b), we have found that the gap energy increase with the increasing of

Table 1. The effective atomic numbers (Z_{eff}) measurements for different concentrations of Zn in $Cd_{1-x}Zn_xTe$.

Alloy	Energy (keV)							
	10	20	30	40	50	60	80	100
CdTe	49.61	49.59	49.62	51.20	51.22	51.23	51.21	51.17
$Cd_{0.75}Zn_{0.25}Te$	48.30	48.31	43.22	48.41	48.43	48.44	48.45	48.45
$Cd_{0.50}Zn_{0.50}Te$	46.76	46.80	39.12	46.09	46.12	46.14	46.16	46.17
$Cd_{0.25}Zn_{0.75}Te$	44.91	44.97	36.28	44.14	44.17	44.20	44.23	44.23
ZnTe	42.67	42.73	34.20	42.47	42.51	42.54	42.57	42.56

Table 2. The effective electron numbers ($N_{eff} * 10^{23}$) measurements for different concentrations of Zn in $Cd_{1-x}Zn_xTe$.

Alloy	Energy (keV)							
	10	20	30	40	50	60	80	100
CdTe	3.10	3.10	3.10	3.20	3.20	3.20	3.20	3.19
$Cd_{0.75}Zn_{0.25}Te$	3.01	3.02	2.70	3.02	3.02	3.02	3.02	3.02
$Cd_{0.50}Zn_{0.50}Te$	2.92	2.92	2.44	2.88	2.88	2.88	2.88	2.88
$Cd_{0.25}Zn_{0.75}Te$	2.80	2.81	2.26	2.75	2.76	2.76	2.76	2.76
ZnTe	2.66	2.67	2.13	2.65	2.65	2.66	2.66	2.66

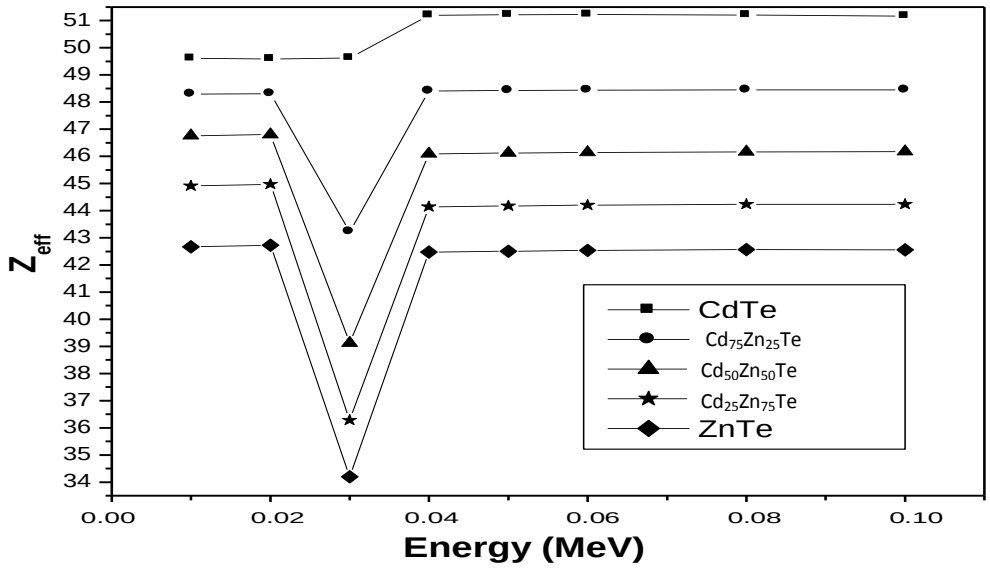

Figure 2. Variation of Z_{eff} with photon energies between (10- 100 keV) for $Cd_{1-x}Zn_xTe$.

concentration of Zn. In our calculations of bulk modulus (B_0), we have found that the maximum of B_0 is at x = 0.75.

Effective atomic and electron numbers

Using our results of mass attenuation coefficient, we have calculated the total atomic cross section (σ_t), the total electronic cross section (σ_e), the effective atomic number (Z_{eff}) and the effective electron number (N_{eff}) of $Cd_{1-x}Zn_xTe$ for photon energies in the range between (10 and 100 keV) using Equations (2, 3), Equations (4 and 5) respectively.

The variation of Z_{eff} and N_{eff} with photon energy for the $Cd_{1-x}Zn_xTe$ alloy is tabulated in Tables 1 and 2 respectively. It is seen that the effective atomic number and the effective electron number have changed with the photon energy in the five compounds. From Figures 2 and 3, both Z_{eff} and N_{eff} are found to be nearly constant

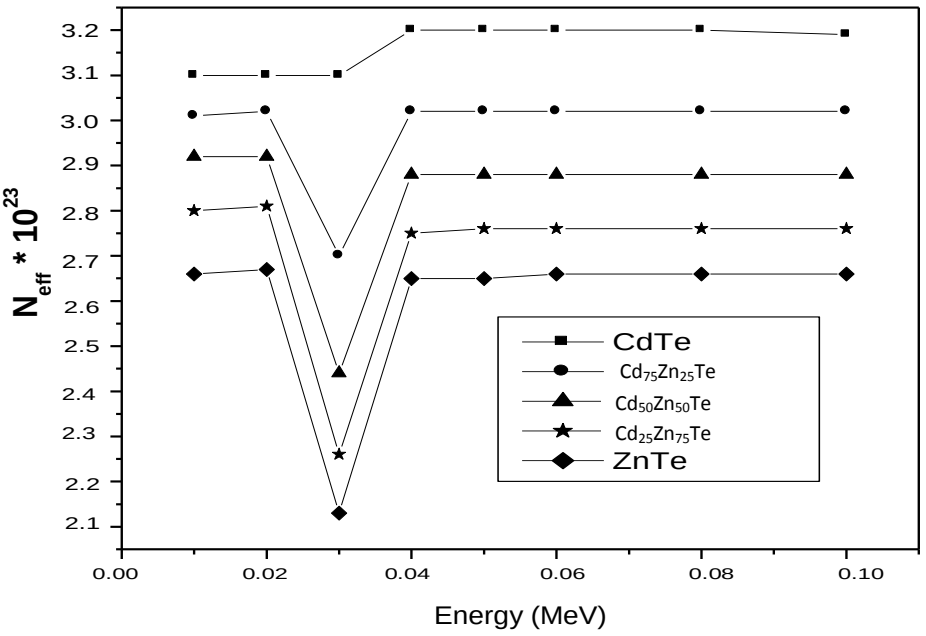

Figure 3. Variation of N_{eff} with photon energies between (10- 100 keV) for $Cd_{1-x}Zn_xTe$.

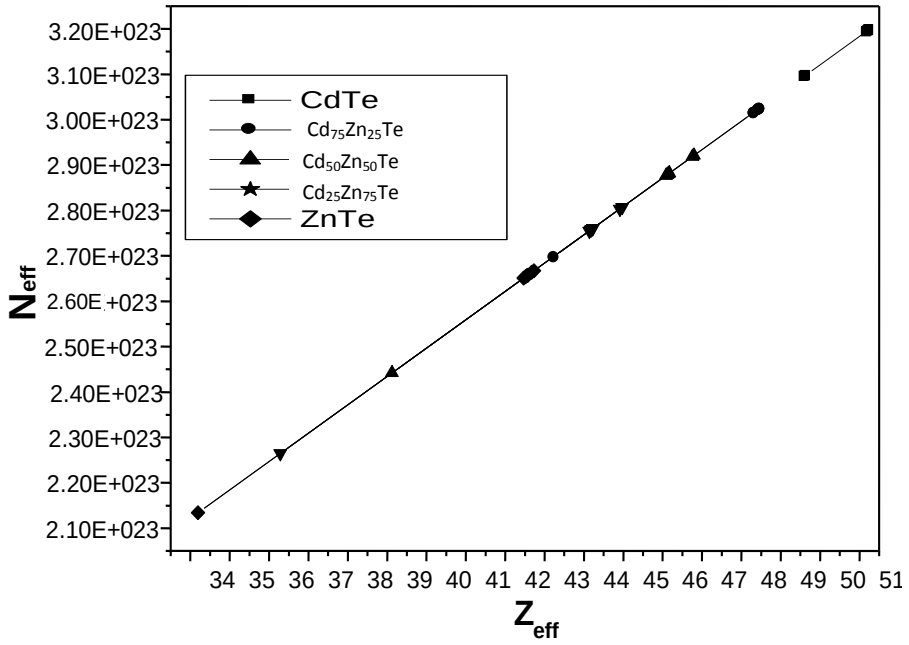

Figure 4. Plots of N_{eff} as a function of Z_{eff} for different concentrations of Zn in $Cd_{1-x}Zn_xTe$ obtained by using XCOM data.

for each compound in the range of energy between (40 and 100 keV). In this energy range, we can classify the Z_{eff} of differentq alloys studied in this work from the biggest in this order: Z_{eff} (CdTe) ≈ 51.21, Z_{eff} ($Cd_{0.75}Zn_{0.25}Te$) ≈ 48.44, Z_{eff} ($Cd_{0.50}Zn_{0.50}Te$) ≈ 46.14, Z_{eff} ($Cd_{0.25}Zn_{0.75}Te$) ≈ 44.19, and Z_{eff} (ZnTe) ≈ 42.53. We have done the same work for the effective electron number (electrons g^{-1}). N_{eff} (CdTe) ≈ 3.20 10^{23}, N_{eff} ($Cd_{0.75}Zn_{0.25}Te$) ≈ 3.02 10^{23}, N_{eff} ($Cd_{0.50}Zn_{0.50}Te$) ≈2.88 10^{23}, N_{eff} ($Cd_{0.25}Zn_{0.75}Te$) ≈ 2.76 10^{23} and N_{eff} (ZnTe) ≈ 2.66 10^{23}. The average Z_{eff} and N_{eff} of $Cd_{0.25}Zn_{0.75}Te$, $Cd_{0.50}Zn_{0.50}Te$ and $Cd_{0.75}Zn_{0.25}Te$ decrease with increasing concentration of zinc.

On the other hand, the Figure 4 shows a linearity

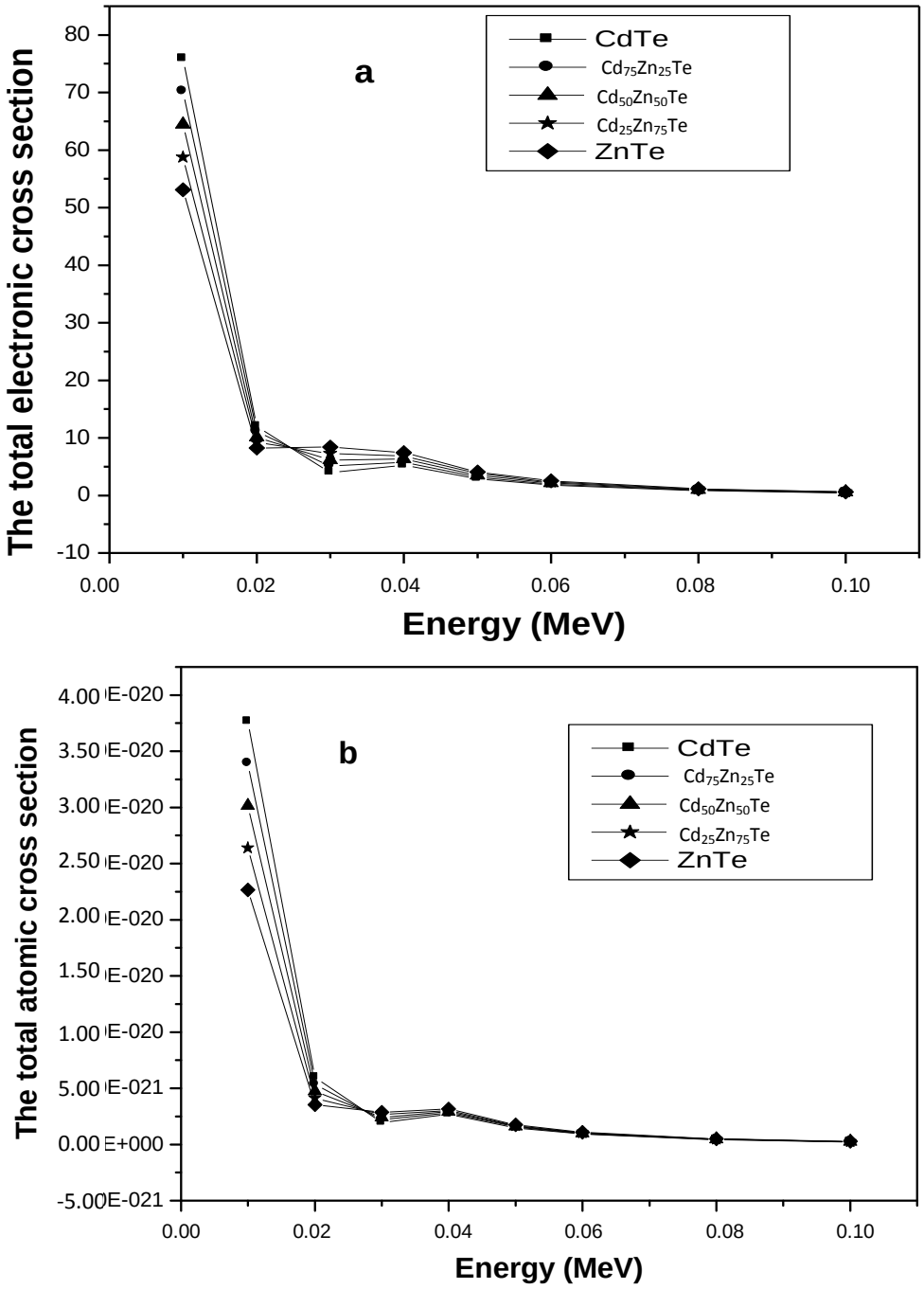

Figure 5. Variation of σ_e (a) and σ_t (b) with photon energies between (10- 100 KeV) for $Cd_{1-x}Zn_xTe$.

between Z_{eff} and N_{eff} which satisfies the Equation (5). we can also see that the five materials have almost the same slope.

The Figure 5 shows that the total atomic cross section and the total electronic cross section became almost constant from 40 keV. In Figure 5b, for the five materials the total atomic cross section decreases with increasing concentration of Zn in energy range between [10 to 40 keV].

Conclusion

Using the theoretical results of XCOM data for the mass attenuation coefficient of $Cd_{1-x}Zn_xTe$ with the different values of x, we have calculated the total atomic and electronic cross sections, the effective atomic number and the effective electron number. In the range of energy between [40 to 100 keV], the effective atomic and electron numbers were found to be constant. This may be

due to the dominance of the photoelectric effect in this range of energy. The linearity between N_{eff} and Z_{eff} is verified.

The effective atomic number and the effective electron number decrease with the increase of the zinc concentration in $Cd_{1-x}Zn_xTe$.

The effective atomic number takes values between the lowest Z = 30 of zinc and the highest Z = 52 of tellure in ZnTe and the ternary $Cd_{1-x}Zn_xTe$. But for CdTe, it takes values between Z = 42 of cadmium and Z = 52.

Finally, this work has been made to estimate the Z_{eff} and the N_{eff} of $Cd_{1-x}Zn_xTe$.

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