

# Optical and structural study of plastic deformation of single crystals CdTe and CdZnTe

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Received: 23 May 2011, accepted: 30 September 2011

## Abstract

*CdTe pure and alloyed with some isoelectronic impurities was found in front of more than twenty years as very promising in optoelectronics. The effectiveness of components based on these materials is strictly related to their quality. It is in this context that our work. The objective in this study is to see the effect of plastic deformation of crystals of CdTe and CdZnTe on crystallographic and optical properties. The investigation methods are X-rays as a means of crystallographic characterization, measurements of UV-Visible spectrophotometry, as means of optical characterization. The main results show that: the best crystal (CdZnTe) before deformation, which shows the highest dislocation density after deformation and increased optical gap, which decreases for CdTe. The effect of dislocations on the optical properties is characterized by a shift of the absorption edge relative to the undeformed state, due to the creation of acceptor centers, which are the neutral hole CdTe and Cd decreased concentration of Zn atoms substituting Cd atoms*

**Keywords:** single crystals, CdTe, CdZnTe, plastic deformation, dislocations, optical gap, UV-visible.

## 1. Introduction :

II-VI semiconductors are materials composed of elements from columns II and VI of the periodic table. In this family, CdTe is the most recommended [1], because of its properties enabling it to detect X and  $\gamma$  [5], and in the field of infra-red, and its use in medical imaging [2,3] and also serves as a substrate for epitaxial infrared detector CdHgTe [4]. CdTe is a direct gap semiconductor, its band structure [6], enables vertical radiative transitions between the valence band and the conduction band. It has a wide band gap of about 1.51eV at room temperature, which is optimal for junction solar efficiency [7]. The cadmium telluride are used to conduct basic physical studies using two characteristics that make them more susceptible to external shocks:

- (i) the binding energy of the exciton oscillator strength and are large, allowing thin optical studies.
- (ii) we can insert elements in the matrix without inducing electrical change, such as Zn, Mn and Hg

Despite efforts to improve the crystalline quality of CdTe, this one still has a density of defects, from physical or chemical considerable. This has prompted researchers to turn to the CdZnTe alloy that provides better crystal quality. An examination of the peculiarities of the electrical behavior, related to the presence of a field of microstrain by dislocations is essential in improving the properties of semiconductors.

All properties of crystals depend in one way or another, the type and density of dislocations, their electronic states and their interactions with other types of defects. In some cases, the influence of dislocations of different types can even be contradictory. It happens to not be able to specify which of the dislocation affects the spectrum of electronic states. To resolve this problem, attention has focused in recent years, using samples with a controlled distribution of dislocations monotypes, study local variations of physical properties of the crystal under the action of individual dislocations. In semiconductors under the influence of dislocations, the mobility of current carriers can vary considerably, and their

concentration, causing changes in electrical and optical properties of these materials.

These changes are manifested by the appearance of energy levels quite new and even areas or by varying the width of the band gap, caused by the dislocation strain field.

## 2. Experimentale

### 2.1 Diffraction X-ray (XRD)

The X-ray diffraction (XRD) allows qualitative and quantitative analysis of the material to the condensed state.

The shape of the diffraction peaks can be related to the crystalline microstructure. Knowledge of the positions of diffraction peaks and intensities of diffracted beams allow the identification of phases present, the measurement of residual stresses, the lattice parameter, grain size and the study of textures. Analyses of X-ray diffraction were performed using a Siemens D5000 diffractometer. The source used is a copper anticathode operating under a power of 1200 W (30 kV and 40 mA).

### 2.2 Optical spectroscopy ultraviolet-visible

In this section we will define the coefficient of optical transmittance and give its physical meaning, as we will describe the method of determining the optical gap  $E_g$  of the material [8].

#### 2.2.1 The transmittance spectra

The transmission coefficient, or transmittance  $T$ , is defined as the ratio of the transmitted light intensity to the intensity of incident light [9].

For the transmittance curves, our samples of CdTe were deposited on glass substrates. These are essential, because it does not absorb light in the spectral range studied. A substrate blank in the reference beam spectrophotometer was used. For plotting the spectra, a computer connected to this unit reproduces the spectra representing the transmittance function of the wavelength of the incident beam.

### 2.2.2 Absorption Spectra

To determine the absorption coefficient ( $\alpha$ ), we used the relation of Bouguer-Lambert-Beer or often simply called, Beer's law [10]:

$$T = e^{-\alpha \cdot d} \quad (1)$$

If one expresses the transmittance T (%), the absorption coefficient is given by:

$$\alpha = \frac{1}{d} \ln\left(\frac{100}{T(\%)}\right) \quad (2)$$

Knowing the thickness of the layer, d, so we can determine the absorption coefficient for each transmittance value which corresponds to an energy. By scanning the entire field of energy, we plotted the variation of absorption coefficient as a function of incident photon energy (hv), an example is shown in Fig.1.

### 2.2.3 Determination of the width of band tail

We carried on a semi-logarithmic variation of absorption coefficient as a function of photon energy. In this region, called the Urbach region, the absorption coefficient can be expressed by the following equation[11].

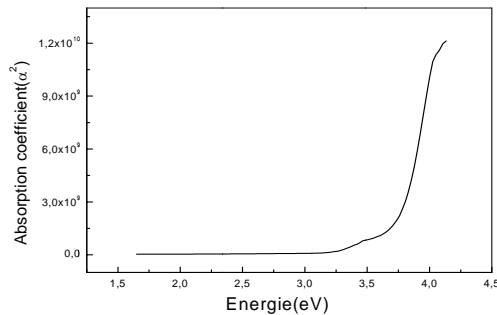


Fig.1 Variation of absorption coefficient

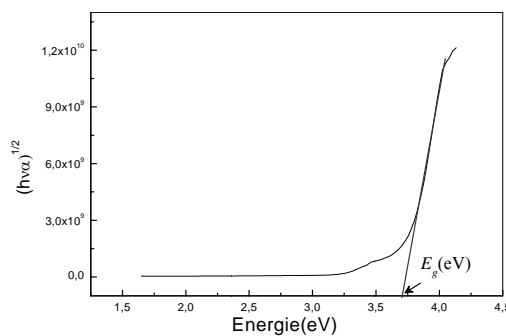


Fig.2 Determination of the energy gap by the extrapolation method from the variation of  $(\alpha hv)^{1/2}$  as a function of hv.

$$\alpha = \alpha_0 \cdot \exp\left(\frac{hv}{E_{00}}\right) \quad (3)$$

By calculating logarithmic slope,  $1/E_{00}$  in this region, we were able to evaluate the disorder of the film  $E_{00}$ , using the inverse of the slope.

### 2.2.4 Determination of the optical absorption threshold

In the area of high absorption ( $\alpha > 10^4 \text{cm}^{-1}$ ), the relationship between the absorption coefficient  $\alpha$  to the photon energy is:

$$(\alpha \cdot hv)^{1/2} = B(hv - E_g) \quad (4)$$

Where B is a constant and  $E_g$  defines the threshold for optical absorption [11,12]. The graphical representation of  $(\alpha \cdot hv)^{1/2}$  a function of energy (Fig. 2) represents a linear part, whose intersection with the axis of energy gives the optical gap  $E_g$ .

### 2.2.5 Working Principle

The optical absorption measurements were conducted at the University of Constantine. We use a tungsten filament lamp (50W) as a white source, that is to say that emit light in a wide range of wavelengths covering the entire spectrum, visible. This light is first filtered by two specially diaphragms, then made parallel by placing the source at the focus of a converging lens. The light transmitted through the sample is spectrally dispersed by the network, then passes through a monochromator and is then detected by a photomultiplier. Measurements are performed at room temperature.

## 3. Result and discuss

### 3. 1. Determination of slip systems

#### 3. 1. 1. Identification of slip system

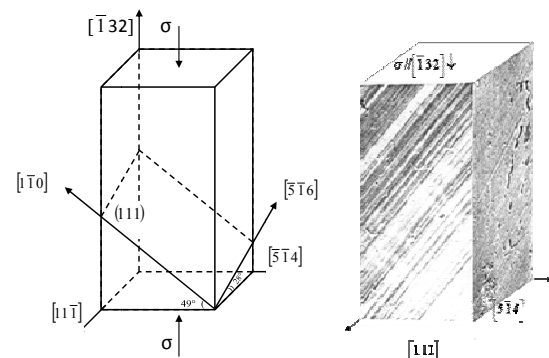


Fig.3 (left): Crystallographic orientations

Fig.4 (right): Images obtained by light microscopy of slip system generated

The specimens for plastic deformation are oriented in such a way as to enable an easy slip system, that is to say having the largest Schmid factor (Fig. 3.a).

For the system with a diamond structure (zinc blende in our case) the slip system in question is the primary system  $[\bar{1}10]$  (111), single system activated under the stress of the stress  $\sigma//[\bar{1}32]$ .

For this slip system Schmid factor is 0.47, Figure 3(a and b) shows the crystallographic orientations and the images obtained by light microscopy of slip system generated.

#### 3. 1. 2 determining the Burgers vector

The slip plane in the case of cubic diamond (111), it is generated by perfect dislocations with the Burgers vectors

$$\frac{a}{2} [110] \quad (13)$$

The system  $[\bar{1}10]$  (111) is generated from corners dislocation characterized by Burgers vector absolute value of the surrounding  $4.56 \text{\AA}$  (Tab.1).

Tab.1: Some parameters of studied samples

Sample	a (Å)	$\ b\ $ (Å)
CdTe Deformed	6,459	4,567
CdZnTe Deformed	6,465	4,571

### 3. 1. 3 Calculation of dislocation density

#### 3.1. 3. 1 width at half maximum of the diffraction peaks and defect density

Much work has been devoted to the study of work-hardened metals. It is possible to link the characteristics of the reflection profile, line width, asymmetry, peak position, size of diffracting domains, density, nature, the width of stacking faults etc. It is a difficult study because the observed effects arise in general from several sources: the line broadening, for example, is due both to the effect size (average size of diffracting domains) and the distorting within areas (presence of stacking faults, etc. ...) [14].

An interesting attempt to link the density of dislocations in the line width was made by P. Gay, P. B. Hirsch and A. Kelly [15]: they interpret the mosaic structure, considering it consists of sub-grains separated by walls of edge dislocations. The angle between two adjacent sub-grains depends on the number of dislocations in the wall and its sign depends on that of dislocations. P. Gay et al assume that the distribution of blocks around a mean position is a Gaussian distribution and consider that the width at half maximum  $\beta$  of reflection profile of this crystal mosaic is equal to the angular width at half height of distribution curve of the small blocks.

From these assumptions, they connect to the  $\beta$  dislocation density

$$\eta_D = \frac{\beta^2}{9b^2} \quad (5)$$

Where  $b$  is the Burgers vector of dislocations. Width  $\beta$  can be deduced from reflection profile recorded using the X-ray diffraction mounting.

Although the quantitative point of view (that is to say the exact determination of the density of dislocations) XRD is not as effective as the method that uses chemical attack bites it remains essential to give a first ruling on the crystalline quality of the crystal to be analyzed.

#### 3. 1. 3. 2 Comparison with experiment

The densities of dislocations before deformation densities are in fact calculated by etching on samples not deformed, where we notice some difference between the three types of samples (Tab.2). We note in particular that the CdTe sample with 4% Zn has a dislocation density less than that observed in pure CdTe.

Tab. 2: Dislocation densities before and after deformation

Sample	$\eta_D$ ( $cm^{-2}$ )	$\eta_D$ ( $cm^{-2}$ )	$\Delta\eta_D$ ( $cm^{-2}$ )
	Before def	After def	
CdTe	$5 \cdot 10^5$	$1,71 \cdot 10^8$	$1,71 \cdot 10^8$
CdZnTe	$8 \cdot 10^5$	$3,57 \cdot 10^8$	$3,57 \cdot 10^8$

#### 3.1.4 Effect of impurity (Zn)

##### 3.1.4.1 Effect on the lattice parameter

The introduction of impurities in the CdTe matrix leads to the variation of lattice parameter, which follows Vegard's law for the whole area of concentration in regard to the Zn impurity (Fig.5)

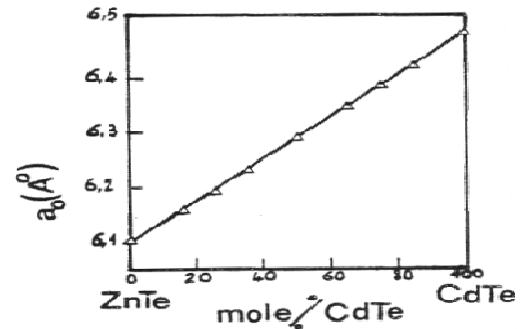


Fig.5 [16]

Tab. 3: XRD results

Sample	$2\theta$ (°)	(h k l)	a (Å)	$\Delta a$ (Å)
C4 not def	23.90	(111)	6,443	0.016
C4 def	23.84	(111)	6,459	
C6 not def	23.98	(111)	6,422	0.043
C6 def	23.82	(111)	6,465	

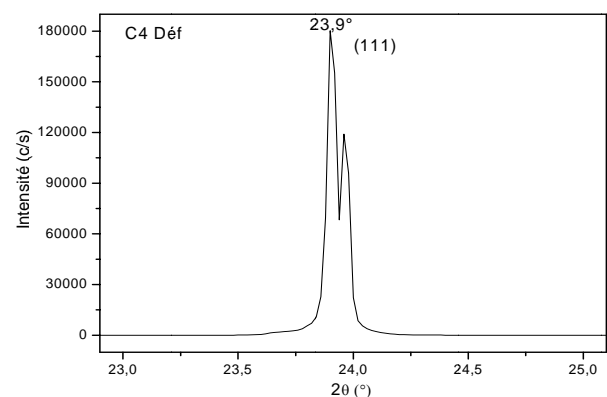
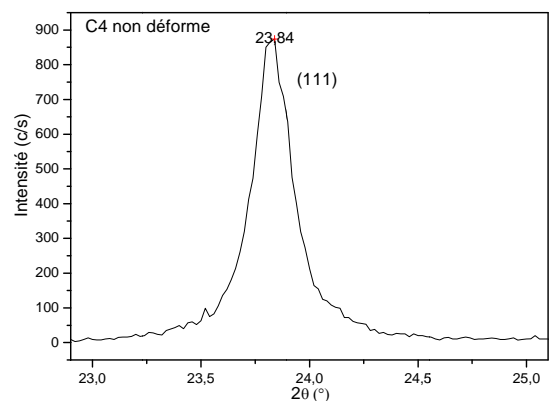


Fig. 6.a XRD spectra of C4 (pure CdTe)

Our work focused on a starting concentration of 4% and the lattice parameter was deduced from XRD spectra (Fig.6.a, b). We notice that after comparison is a small difference probably due to two things:

- The concentration after growth is not the start.
- Growing conditions have allowed us to obtain the empirical variation (tab.4), are not the same used to obtain these materials.

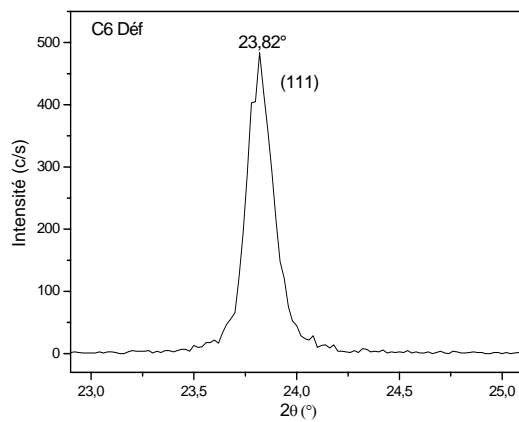
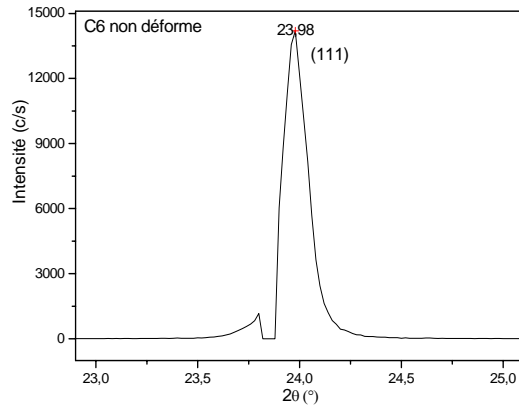


Fig. 6.b XRD spectra of C6 (CdTe with 4% Zn)

Tab.4:

Sample	$a_{exp}$ (Å)	$a_{the}$ (Å)	$\Delta a$ (Å)
C4 CdTe	6.443	6.481	0.038
C6 CdZnTe	6.422	6.456	0.034

3. 1. 4. 2 Effect on the density of dislocations:

The explanation of previous results was provided by K. Guergour and colleagues [17], they assign this reduction to cure provided by the introduction of Zn anchor who makes a line break between two atoms of Zn and subsequently prevents the multiplication of these, other hand experience plastic deformation allowed us to give a quantitative estimate of the density of dislocations caused by the deformation. Table III.2 shows indeed a density of some  $10^8 \text{ cm}^{-2}$  for all samples.

Once it is all very interesting to note that the sample as little dislocated, had the case C6 is one that generates a dislocation density larger, about 10 times that seen on C4.

At the moment there is no plausible explanation for this phenomenon, other more specific studies are needed.

But we note nevertheless that the density of dislocations generated in the samples alloyed with Zn is greater than that of pure material.

3.2 Measurement by UV-Visible

The measurement results are illustrated by (Fig.7,8), these measures helped to track the movement of the absorption edge after deformation.

Tab. 5: Energy gap

Sample	$E_g(\text{ev})$		$\Delta E_g(\text{ev})$
	Not deformed	Deformed	
CdTe	1.476eV	1.448eV	0.028
CdZnTe	1.486eV	1.435eV	0.038

One interesting observation that can be deduced on the comparison of samples not deformed them, where one can see:

- The displacement of the absorption edge towards higher energies for CdTe alloyed with Zn, which means an increase in energy of the width of the band gap. This is confirmed otherwise [17].

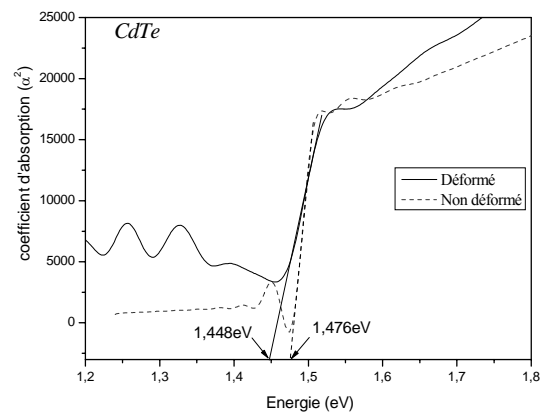


Fig.7 UV-Visible spectra for pure CdTe

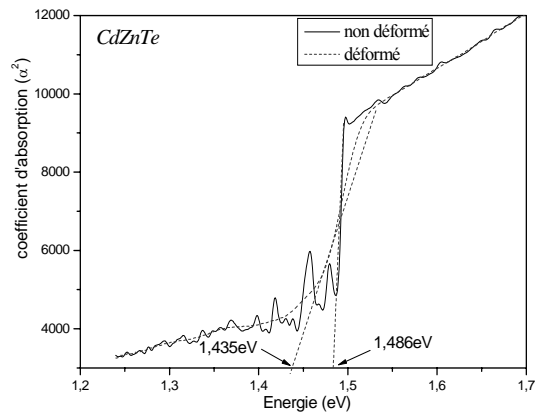


Fig.8 UV-visible spectrum for CdZnTe

- On the deformed state, we notice a decrease in the absorption edge  $E_g$  compared to the undeformed state, up to 38 meV.

These results lead us to emphasize that: in general, there was a decrease in energy, given by the absorption edge, due to the creation of level above the top of the valence band, c that is to say that the plastic deformation causes the creation of acceptor centers with their energy close to  $E_v$ . In other words the absorption is below the energy-related acceptor center created by plastic deformation.

The narrowing of  $E_g$ , as regards CdTe is due by K. Guergour et al [17] to the creation of gaps of Cd neutral after work

photoluminescence on samples deformed by Vickers microindentation.

The same authors attribute the decrease of  $E_g$  in the case of CdZnTe, decrease the concentration of Zn atoms attracted to the dislocations created by plastic deformation.

#### 4. Conclusion

CdTe pure and alloyed with some isoelectronic impurities was found in front of more than twenty years as very promising in optoelectronics.

The effectiveness of components based on these materials is strictly related to their quality. It is in this context that our work.

The objective in this study is to see the effect of plastic deformation of crystals of CdTe and CdZnTe, the crystallographic and optical properties.

The investigation methods are X-ray diffraction (XRD) as a means of structural characterization and measurements of UV-Visible spectrophotometry, as a means of optical characterization.

The main results show that:

The best crystal (CdZnTe) before deformation, is the one with the highest dislocation density after deformation and higher optical gap.

The effect of dislocations on the optical properties is characterized by a shift of the absorption edge relative to the undeformed state, due to the creation of acceptor centers, which are the gaps neutral CdTe and Cd decreased concentration of Zn atoms substituting Cd atoms

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