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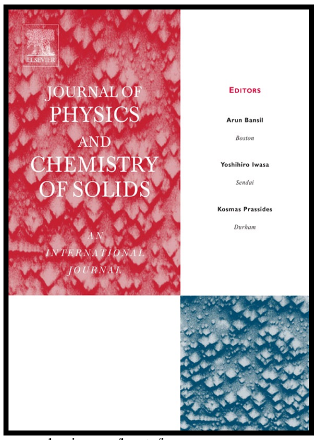

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PII: S0022-3697(16)30272-4
DOI: http://dx.doi.org/10.1016/j.jpcs.2016.07.009
Reference: PCS7811

To appear in: *Journal of Physical and Chemistry of Solids*

Received date: 10 April 2016
Revised date: 10 June 2016
Accepted date: 6 July 2016

Cite this article as: F. Lmai, R. Moubah, A.El. Amiri, A. Boudali, E.K. Hlil anc H. Lassri, Effect of plastic deformation on the optical and eletrical properties i $Cd_{0.96}Zn_{0.04}Te$ single crystals, *Journal of Physical and Chemistry of Solids* http://dx.doi.org/10.1016/j.jpcs.2016.07.009

Effect of plastic deformation on the optical and eletrical properties in $Cd_{0.96}Zn_{0.04}Te$ single crystals

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Abstract

Using UV-visible, photoluminescence, electrical measurements and *ab*-initio calculations, we study the effect of introduced dislocations on the optical and electrical properties in $Cd_{0.96}Zn_{0.04}Te$ crystals. To generate dislocations, a plastic deformation on the Cd(111) and Te $(\bar{1}\,\bar{1}\,\bar{1})$ faces was induced. It is shown that the plastic deformation results in: i) a decrease in Zn concentration in the deformed regions, which is higher on the Cd face, ii) decrease in the band gap energy, iii) an increase of acceptor concentration, and iv) the leakage current is higher on the Te face. Calculation of barrier height has led to identify the dominant defect, which is the complex Cd vacancies, acceptor center $[V_{Cd}, A_{Cd}]$ on the Cd face and V_{Te} on the Te side, respectively. Electronic structure calculations based on full potential linearized augmented plane waves (FPLAPW) method were performed as well and have shown that the optical band gap energy decrease upon deformation can be understood by the decrease in Zn content in the deformed regions.

Keywords: Impurity and defect levels; II-VI Semiconductors; Optical properties; Photoluminescence; Structure electronic calculation
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1. Introduction

CdTe is a well-known semiconductor and has been extensively studied in recent years due to its high potential applications in *x*- and γ-ray detectors [1,2]. Generally, the use of CdTe in spectroscopic detectors requires a high crystalline quality of the material [3,4]. Doping CdTe crystals with Zn atoms appears to be a good route for improving the crystallinity [5]. Furthermore, it permits to increase the electrical resistivity [6,7]. On the other hand, it is known that the structural defects can affect significantly the physical properties of materials [8]. In case of CdTe, most of these defects are situated in the dislocation network, which can be due to growth process, e.g., local nonstoichiometry and dislocation movements. Other defects may also appear close to the walls of the ampoule at the stage of the solidification process of crystals. In this work, we investigate the influence of an induced plastic deformation on the optical and electrical properties of $Cd_{0.96}Zn_{0.04}Te$ crystals using photoluminescence, UV-visible, electrical measurements and *ab*-initio calculations. The mechanical deformation was induced by means of Vickers's microhardness method. The effect of a bad crystalline quality (deformed crystals) on the properties of devices is reported. In particular, we focus on the Cd(111) and Te $(\bar{1}\,\bar{1}\,\bar{1})$ faces because there is a polarity effect in the <111> direction. Furthermore, electronic structure calculations based on full potential linearized augmented plane waves method were performed as well and computed band gap energies were compared to our experimental data.

2. Experiment and electronic structure calculations

$Cd_{0.96}Zn_{0.04}Te$ single crystals were prepared by horizontal Bridgman method ingots. In order to get different faces (Cd and Te), the as-grown crystals were mechanically polished using diamond paste with a 0.25 µm grain size, then they were mechano-chemically polished using bromine methanol solution [9].The structural and