Chalcogenide Letters Vol. 6, No. 8, September 2009, p. 393 – 398

GROWTH AND CHARACTERIZATION OF ZnTe CRYSTALS GROWN BY PHYSICAL VAPOR TRANSPORT TECHNIQUE

K. D. PATEL, G. K. SOLANKI, J. R. GANDHI, S. G. PATEL
Department of Physics, Sardar Patel University, Vallabh Vidyanagar – 388120, India

Crystalline Zinc Telluride having a direct wide band gap has attracted many researchers due to its important luminescence properties. In this paper authors present their study on the growth of ZnTe crystals by Physical Vapor Transport Technique. The EDAX analysis has been carried out to determine the stoichiomatric proportion of Zn and Te in the grown mass. From X-Ray diffraction (XRD) studies the structure of the grown crystals were found to be cubic. The optical characterization has been done by means of UV-VIS-NIR spectrophotometer and optical band gap has been calculated.

(Received September 11, 2009; accepted September 15, 2009)

Keywords: Zinc Chalcogenides, ZnTe crystals, Physical vapor Transport, EDAX, XRD

1. Introduction

Zinc Chalcogenides (ZnS, ZnSe ,ZnTe) are the wide band gap II-VI compounds. II-VI compounds possess high iconicity (0.77, 0.63, 0.49 respectively for ZnS, ZnSe ZnTe) [1] of chemical bond, therefore they have smaller energy of formation of vacancies and these accounts for the large II-VI nonstoichiometry, and also they are very sensitive to any strain. Thus high ionic character of these compounds makes it difficult to control the growing interface both from melt and vapor phase. The wide band gap II-VI compounds are the promising materials for their use in many optoelectronic applications. ZnTe having a direct band gap of 2.26 eV at room temperature is one of the most important among them. Due to its wide band gap, it can effectively emit light of 540 nm, which is the spectral region having maximum sensitivity for the human eyes. Thus this is the promising material for its application in pure Light Emitting Diode and Laser Diode [2, 3]. It also has a potential application as IR optics, crystal pieces for vacuum deposition and window material for CdTe based solar cells [4, 5]. Because of its large electro-optic coefficient among most of the compound semiconductors it can be used as a terahertz detector [6-9]. ZnTe crystals are non-toxic, moisture resistant, and they conserve working parameters after gamma irradiation up to 107 Rad and continuous heating up to 400 K, therefore, they are widely used for multipurpose ionizing radiation detectors of Scintillator-sillicon photodiode type to be used for radiation monitoring, medical and technical tomography, X-ray medical devices, non destructive testing systems and custom inspection, spectrometry of alpha and beta radiation as well as for soft X-rays [10,11]. Crystallization from the vapor phase has an advantage over a melt growth, particularly for II-VI compounds as they have high melting temperature which can make the melt growth process difficult to be handled. Physical vapor transport acts as a purification process because of difference in vapor pressure of native elements and impurities [12, 13]. Though to increase the transport rate and to reduce the growth temperature, the transporting agent (I_2) can be employed in case of Chemical Vapor Transport technique [14] but the disadvantage is the high level of unintentional doping of transporting agent (I_2) [15-17].

To increase the life time and to improve the performance of the electro optical devices based on ZnTe compound it is necessary to improve the basic properties of the grown compound.

Here the authors present their work on growth and structural characterization of ZnTe crystals grown by PVT technique.

2. Experimental procedure

Preparation of ZnTe charge

A 7.5 gm of mixture of Zn (purity 99.99 %, Make: Fluka Chemic GmbH) and Te (Purity 99.99 % Make: Chiti Chem corp. Baroda) was filled in a dried ampoule of 25 mm of diameter and 250 mm of length in stoichiometric proportion. Before filling of the materials the ampoule was properly washed and rinsed with distilled water. The ampoule was than sealed at pressure 10^{-5} Torr. This sealed ampoule was placed in a dual zone furnace to obtain a charge of ZnTe at constant reaction temperature. Ampoule was maintained at constant temperature of 1073 K for 36 hours and than cooled down to room temperature. The charge thus prepared was rigorously shaken to ensure the proper mixing of the constituents. The EDAX analysis has been carried out to determine the proportion of Zn and Te in the charge.

Crystal Growth Process

The synthesized compound was transferred into another quartz ampoule and was sealed at pressure of 10^{-5} Torr. This sealed ampoule was now loaded in to two zone furnace for crystal growth. The source zone was kept at higher temperature compared to that of the growth zone for a finite period of time. In order to avoid any influence of mechanical vibration to the crystal quality, ampoule was kept motionless during the growth process. After definite time period, it was slowly cooled down at the rate of 20 K /hour to the room temperature. To optimize the gradient between the source and growth zones of furnace, several runs were taken. The process was initially started with the temperature gradient of 100 K. This gradient was then reduced to 10 K after investigating the results. Thus finally after four runs, the gradient was set to 50 K that resulted in formation of small crystals. The selection of upper temperature and the gradient of temperature between source and growth zones were made on the basis of an extensive literature survey. Complete details of the growth parameters for growth cycles of about 168 hours are shown in Table-1. The grown crystals are also shown in the figure -1.

For X-Ray diffraction study, several small crystals were finely ground with the help of an agate mortar and filtered through 100-micron sieve to obtain grains of nearly equal size. X-Ray diffractograms were taken with Philips X-Ray diffractometer employing CuK_{α} radiation. The patterns obtained are shown in figure – 2. The absorption spectra were obtained by means of UV-VIS-NIR spectrometer in the range of 200 – 3000 nm.

3. Results and discussion

The result of the EDAX analysis confirms the stoichiometric proportion of Zn and Te for the grown crystals. The X-Ray diffractogram of ZnTe shows a well defined sharp diffraction peaks as shown in figure-2, which indicates a good crystallinity of the specimens. The (hkl) values corresponding to prominent reflections, d values, peak width and peak intensities are shown in Table-3 along with the particle size for a number of reflections. The values of lattice parameters a,b,c, the volume (V) and X-ray density (ρ) obtained from the analysis of the diffractogram of the crystal are presented in Table -2. The values of lattice parameters obtained for ZnTe crystals were found to be in agreement with the same reported earlier. The obtained values of lattice parameters indicate a cubic structure of the sample. The particle size has been evaluated using Scherrer's formula

$$t = \frac{K\lambda}{\beta \cos\theta} \tag{1}$$

Where t is the crystallite size as measured perpendicular to the reflecting plane, K is the Scherrer constant whose value is taken to be unity assuming that the particles are of spherical shape, λ is the wavelength of X-ray radiation, β the half width intensity which is measured in radians and θ is the Bragg angle.

The optical absorption spectra were recorded over the spectral range of 200 nm -2000 nm. The optical absorption spectra of as grown crystals are shown in Figure-3. For the determination of band gap the best fit of all the experimental points were observed in $(\alpha h\nu)^2$ vs $h\nu$ plot as shown in Figure-4 for ZnTe. The value of direct band gap as determined from this plot is found to be 2.20 eV for ZnTe crystals.

Table 1. Growth conditions for various cycles for ZnTe crystals.

Run No.	Temperature Distribution			Result
	Hot Zone (K)	Cold Zone (K)	Diff. (K)	
1	1150	1050	100	Ingots
2	1150	1070	80	Ingots
3	1150	1080	70	Ingots
4	1150	1090	60	Ingots
5	1150	1100	50	Crystals of 4mm× 3mm× 2mm size (App.)

Table 2. X-ray diffraction data for ZnTe crystals grown by PVT.

(h k l)	d-spacing (Å)	Peak Width (°2θ)	Peak Intensity (Counts/second)	Particle size (Å)
(1 1 1)	3.5234	0.21	1281.2	387.86
(2 2 0)	2.1573	0.21	1473.61	405.19
(3 1 1)	1.8402	0.28	1019.3	312.56
(4 0 0)	1.5263	0.35	138.28	263.04
(4 2 2)	1.2456	0.42	549.37	240.76
(3 3 3)	1.1748	0.28	232.79	375.67
(4 4 0)	1.0790	0.21	106.06	540.41
(5 3 1)	1.0315	0.21	511.37	569.07
(4 4 2)	1.0171	0.21	41.03	579.47

Table 3. Crystallographic data of ZnTe crystals grown using PV.

Parameter	JCPDS data (PDF No: 150746)	Present Work
a =b=c (Å)	6.1026	6.0975
Unit cell Volume V $(Å)^3$	227.27	226.70
X-ray density ρ (gm . cm^{-3})	5.64	5.65

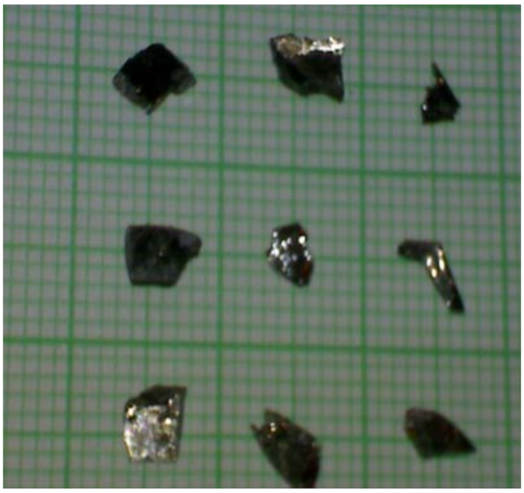

Fig. 1.As grown crystals of ZnTe.

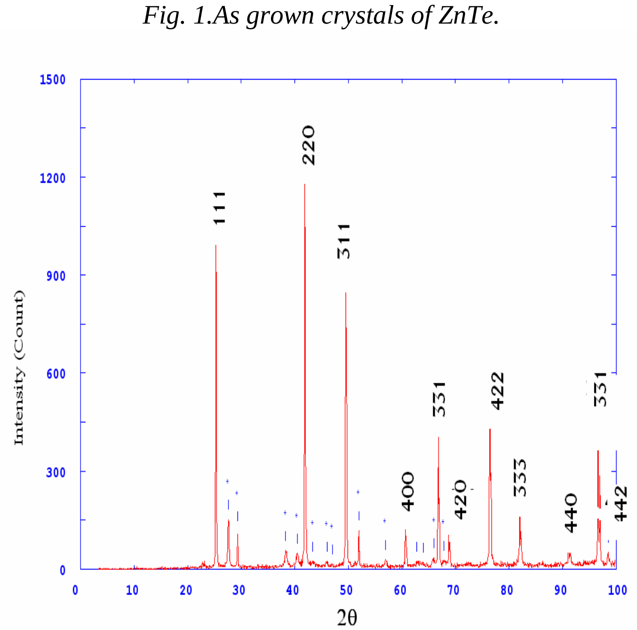

Fig. 2. X-ray powder diffractogram of ZnTe

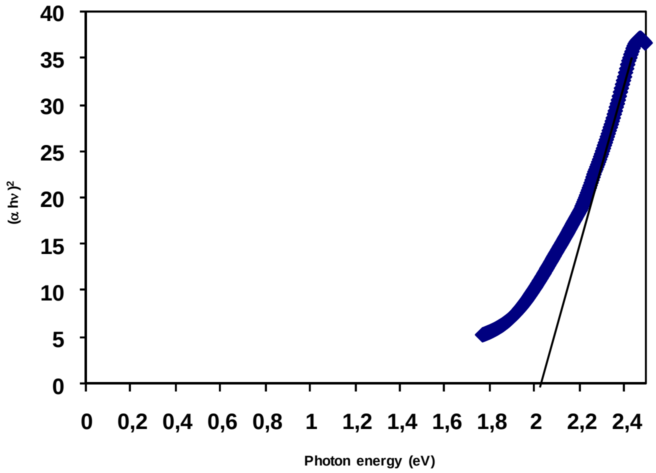

Fig.-3. Optical spectra of ZnTe crystals

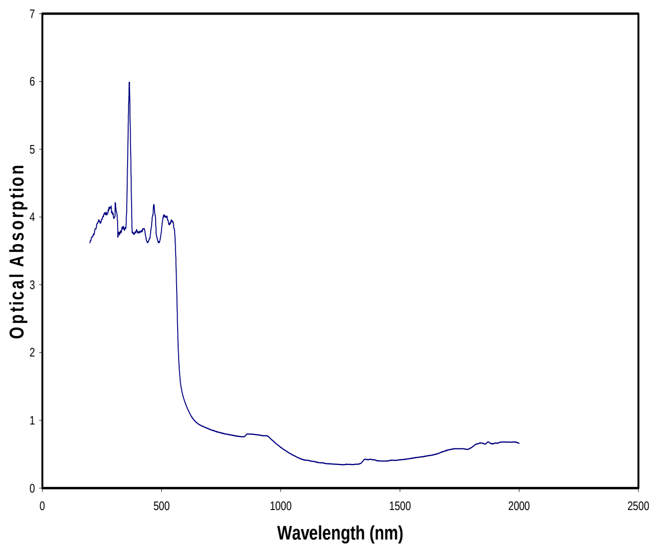

Fig. 4. $(\alpha h\nu)^2$ *vs* $h\nu$ *plot of ZnTe crystal.*

4. Conclusion

Physical Vapor Transport Technique is suitable for the growth of ZnTe crystals. It is found that the temperature gradient of 50 K is appropriate for the growth of small yellowish shining crystals. The EDAX study confirms a stoichiometry of the grown crystals. The X-Ray diffraction analysis confirms a cubic structure of grown crystals. The optical band gap of the as grown crystals is found to be 2.20 eV.

References

[1] R.Trtiboulet, J.O.Ndap, A.Ei.Mokri, A. Tromson and A. Zozime, Journal De physique IV **volume 5,** C3-141-148(1995)

[2] Wu-Yih Uen, Shium-Yi Chou, Hwa-Yuhshin Sen-Mao Liao, Shan-Ming Lan Material Science and Enagineering **B 106 ,** 27-32 (2004)

[3] Nishito M., Hayashida K, Guo Q., Ogawa H. Applied Surface Science, **223,** 169-170 (2001)

[4] Takahicro Ishizaki, Nagahiro Saito, Osamu Takai, SAhuichi Asakwra, Kaori Goto, Akio Fuwa Elactrochimica Acta **50**, 3509-3516 (2005)

[5] PVS Meyers, Proceedings of 7th Commission European Communities Conference on Photovoltaic Solar Energy, Reidel, Dordrecht, Netherlands, page-1121 (1986)

[6] Ashai T., Yabe T., Sato K., Arakawa A. Journal of Alloys and compounds **371**, 2-5 (2004)

[7] Q.Wu. Hewitt, X-C Zhang Applied Physics Letters **77**, 176 (2000)

[8] Herrmann M., Sakai K., TanM. i, Fukasawa R.. Proceedings of 8th International Conference on Terahertz Electronics P.185 (2000)

[9] Takahash H., Hosoda M. Applied Physics Letters **77**, 1085 (2000)

[10] Marketech International Inc. www.mkt-intl.com

[11] Cardley Crystals Inc. www.cardley-crystals.com

[12] Ching –Hua Su and Yi-Gao Sha Current Topics in Crystal Growth Res. (NASA-CR-204722) **2** (1995)

[13] Lauck R. Muller-Vogt G. & Wenchi W Journal of Crystal Growth **74**, 520 (1986)

[14] Hartmaan H. Journal of Crystal Growth **42**, 144 (1977)

[15] Catano. A. & Kum Z.K. Journal of Crystal Growth **33**, 324 (1976)

[16] Koyoma ,T. Yodo,T. Aka, H. Yamashita K. & Yamasakai T. Journal of Crystal Growrh **91**, 639 (1988)

[17] Fujita S. Mimoto, H. Takeba H. & Noguchi T. Journal of Crystal Growth **47**, 326 (1979)