

Study on Cd vacancy in CdZnTe Crystal by Positron Annihilation Technology

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2013 J. Phys.: Conf. Ser. 419 012040

(<http://iopscience.iop.org/1742-6596/419/1/012040>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 218.22.21.3

This content was downloaded on 26/11/2014 at 12:07

Please note that [terms and conditions apply](#).

Study on Cd vacancy in CdZnTe Crystal by Positron Annihilation Technology

Weiwei Liu, Jiahua Min*, Xiaoyan Liang, Jijun Zhang, Xiaoxiang Sun, Linjun Wang, An Ran, Bangjiao Ye

Department of Electronic Information Materials, School of Materials Science and Engineering, Shanghai University, 149 Yanchang Road, Shanghai 200072, China

E-mail: minjh@shu.edu.cn

Abstract. Cd vacancies in cadmium zinc telluride (CdZnTe) crystals have an important effect on the crystal properties. In this paper, position distribution and concentration change of Cd vacancy in CdZnTe crystal grown by the temperature gradient solution growth (TGSG) were investigated by positron annihilation technology (PAT), which was based on the potential energy distribution and probability density of the positron in the crystal. The results showed that, the density of Cd vacancy increased obviously from the first-to-freeze to stable growth of the ingots, while decreased along the radial direction of the ingots.

Keywords: CdZnTe; Cd vacancy; positron annihilation Technology (PAT)

1. Introduction

Owing to its large average atomic number, wide band gap, high resistivity, and good electron transport properties, Cadmium Zinc Telluride (CdZnTe) has become one of the most exploited materials for x-ray and gamma-ray radiation detection at room temperature, which has broad prospects in medicine, space science, airport, port security, nuclear waste monitoring and other applications of nuclear technology^[1-3].

High resistivity, good integrity of CdZnTe monocrystal is essential for high-performance detectors. However, the relatively high equilibrium vapor pressure of Cd easily leads the lack of Cd in CdZnTe single crystals, therefore imperfections such as Cd vacancies, Te inclusions, and Te antisite are included in the process of crystal growth^[4,5]. The above problems would affect the stoichiometric ratio of CdZnTe monocrystalline and cause crystal component segregation, resulting in many defects in the crystal as-grown, which is detrimental to the

detection performance of the device, and thus the application of CdZnTe monocrystal.

Now there are a lot of methods to analyze the defects of CdZnTe single crystal, such as photoluminescence (PL), electron paramagnetic resonance (EPR), electron microscopy (SEM and TEM) and so on. However, these methods are difficult to obtain the information about the microscopic structure on the atomic scale. In the past 20 years, positron annihilation technology has been widely used to study neutral vacancy-type and negatively charged vacancy-type defects in the solid. As the neutral vacancy and negatively charged vacancy will become the captured trap of positive electrons, so that the positive electrons which have been injected in will be captured by the neutral vacancy and negatively charged vacancy after thermalization and diffusion. Then the positive electrons will annihilate and release two γ photons. The characteristics of defects in the solid can be analyzed by the information carried by the γ photons.

As we all know that the rate of positron annihilation is proportional to the electron concentration of the place where the annihilation appears. There are different positron lifetime according to the annihilation appears at the different types of vacancies^[6]. The experimental data of positron annihilation can not only give the relationship between lifetime and temperature, but also identify the charge state and the ionization energy of the defect.

The CdZnTe crystal in this research was prepared through the temperature gradient solution growth method (TGSG) in the lower growth temperature. Furthermore, the radial and longitudinal distribution of Cd vacancies can be analyzed by the positron annihilation technology to obtain the properties of defects.

2. Experiment

2.1 Experimental samples

Test samples are prepared with the CdZnTe crystal made through the method of temperature gradient of the solution growth (TGSG), 14 groups of wafers were cut from the same ingot, and sequentially each sample was made of the adjacent two wafers with the size of 10mm×10mm×1mm on average. In order to remove the surface oxide layer and the stress layer, thus reduce the interference during the measurement process, the wafers were mechanically and chemically polished with Al₂O₃ powder and bromine methanol of 2 to 3%.

Table 1. The relative position parameter of the sample on radial direction test
(r=0: the center of ingot)

sample	logitudinal direction (mm)	radial direction (mm)	sample	logitudinal direction (mm)	radial direction (mm)	sample	logitudinal direction (mm)	radial direction (mm)
a1#	Z=10	r= -10	b1#	Z=20	r= -10	c1#	Z=30	r= -10
a2#	Z=10	r= 0	b2#	Z=20	r= 0	c2#	Z=30	r= 0
a3#	Z=10	r= 10	b3#	Z=20	r= 10	c3#	Z=30	r= 10

Table 2. The relative position parameter of the sample on logitudinal direction test

sample	4#	5#	6#	7#
logitudinal direction(mm)	Z=5	Z=15	Z=25	Z=35

2.2 positron annihilation lifetime test

The Positron Annihilation test was carried out using ORTEC positron spectrometer , with ^{22}Na as the positron source. The instrument has a FWHM of 210ps, and its total number of each lifetime spectrum is 10^6 .

3. Results and Discussion

When the point defects in the solid are capturing the positron, the main process is 2γ annihilation. For the two-state capture model, computer fitting can be used on positron annihilation lifetime spectroscopy curve decomposition. We have used General POSITRONFIT fitting procedure, obtained two life values τ_1 , τ_2 and the intensities were I_1 , I_2 , respectively. Therefor the trapping model average life τ_m and capture rate κ of the two-state positron was as follows:

$$\begin{aligned} I_1 + I_2 &= 1 \\ \tau_m &= \tau_1 I_1 + \tau_2 I_2 \\ \kappa &= I_2 (\tau_1^{-1} - \tau_2^{-1}) \end{aligned} \quad (1)$$

Table 3. The positron annihilation lifetime(PAL)of CdZnTe crystal in the radial direction

	a1#	a2#	a3#	b1#	b2#	b3#	c1#	c2#	c3#
τ_1/ps	214.5	215.2	214.6	215.1	216.3	215.3	216.4	217.4	216.5
τ_2/ps	353.7	353.6	353.9	354.5	354.4	354.6	355.6	355.1	360.3
$I_1/\%$	80	81.4	79.7	81.4	81.6	81.1	82.4	83.4	82.5
$I_2/\%$	20	18.6	20.3	18.6	18.4	18.9	17.6	16.6	17.5

Table 4. The positron annihilation lifetime(PAL)of CdZnTe crystal in the logitudinal direction

	τ_1/ps	τ_2/ps	$I_1/\%$	$I_2/\%$	τ_m/ps	$\kappa/\text{s}^{-1} \times 10^8$
4#	212.3	353.6	79.4	20.6	233.1	2.77
5#	215	354.9	82.3	17.7	239.8	3.24
6#	215.6	356.1	81.7	18.3	248.12	4.25
7#	217.5	367.2	76.8	23.2	254.8	4.89

Positrons generally annihilate freely in the idealized crystal lattices. If vacancies or micro-structural defects (such as vacancy clusters and dislocations) present in the medium, positrons can be easily captured by defect, forming captured states. Usually species of point defects including vacancies, interstitial atoms, and substitutional defects may exist in CdZnTe crystals.

As a general rule, positrons can be captured by negative ions, neutral impurity and dislocations, forming weak bound states in CdZnTe crystals as well. But these defects can be ignored, because they have little effect on positron lifetime. Additionally, interstitial atoms, substitutional defects and positron can also trap positrons shallowly. The positron annihilation lifetime in these states is similar to the bulk material^[7], which have a relatively small influence on positron lifetime. So for CdZnTe single crystal, the vacancy is the main capture potential for positrons. Te vacancies in CdZnTe crystals do not influence the lifetime^[8], because they are positively charged and can not capture positron.

However, Cd vacancies are negatively charged and can be the trapping center of the positive electrons, so that they will have the greatest impact on the lifetime of positron. Since the Zn occupy and randomly distribute at the position of the Cadmium which forms negatively charged cationic vacancies, so that Zn in CdZnTe single crystal is just one kind of substitution of Cd. In a word, all cationic vacancies are naturally equivalent.

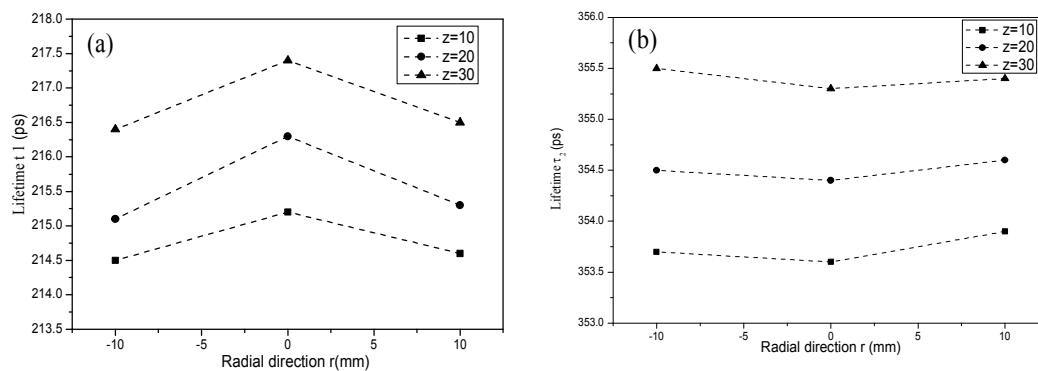


Figure 1. The relation between the positron annihilation lifetime τ_1 (a) , τ_2 (b) and the radial direction parameters

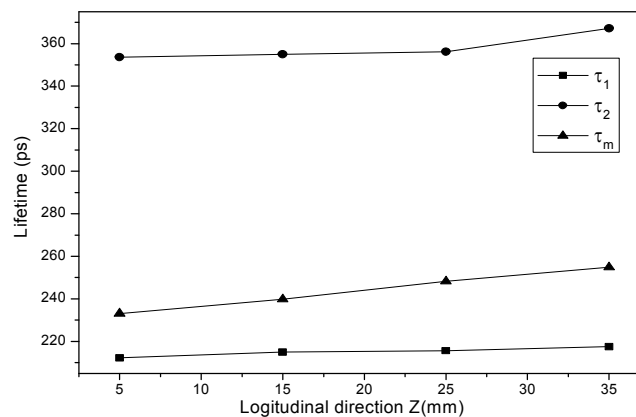


Figure 2. The relation between the positron annihilation lifetime τ_1 、 τ_2 , the average lifetime and the logitudinal direction parameters

In Fig. 1, it can be seen that in the radial direction, compared with the parameter τ_1 , the comprehensive lifetime of the free state of positron and the captured annihilation of single vacancy decreased, both the parameter τ_2 which is the long lifetime value of comprehensive lifetime related to the vacancy cluster and the defects of microstructure and the average lifetime of τ_m ^[9] related to the sizes of defects and concentration have no dramatical changes.

Due to the change of the content of Zn component^[10,11], the Cd vacancies in the center are more than that on the edge. In order to prove this relationship, scanning electron microscopy spectrometer(SEM) is used to test three samples CZT1,CZT2 and CZT3, which were at different positions along the growth axis direction in the same ingot, so that the content of Zn components can be measured evenly spaced along the radial direction and the results are shown in Fig. 3 (r=0: the center of ingot).

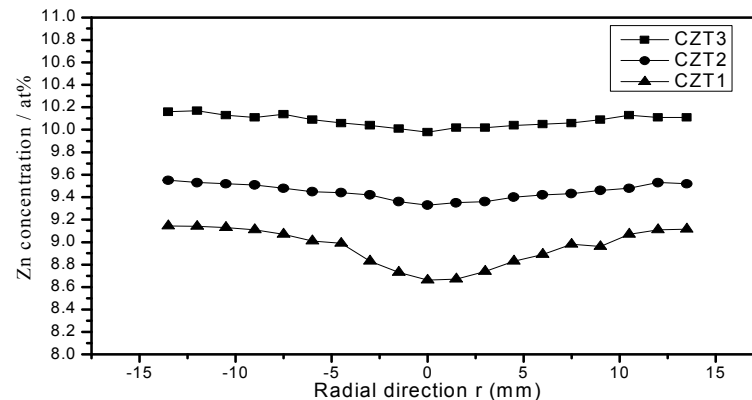


Figure 3. Zn component distributions in radial and axial of the crystals

As shown in Fig. 3, the content of Zn component increases along the radial axis in the crystal, but the lifetime τ_1 shows a contrary tendency. Therefore it is found that the concentration of Cd vacancy will decrease with the increasing of Zn component. In Fig.3, it is clear that τ_1 gradually increases in the direction of the crystal growth, meanwhile, τ_2 , τ_m and κ also increase. All that is resulted from the increasing of single vacancies along the growth direction part of them aggregate or coalesce and become bigger, so the relative vacancy cluster increase which is not only affected by the change Zn component. At the same time, since the liquid-solid interface is concave at the end of crystal growth which can easily promote the production of dislocation, the crystal quality declines. It is one of the impact factors which cause the enlargement of lifetime.

From Table 3 and 4, τ_1 always fluctuate around 216ps, so it can be concluded that positron free state annihilation life of CdZnTe crystal grown by the temperature gradient solution growth (TGSG) is about 216ps.

4. Summary

In this paper, the concentration and distribution of Cd vacancies in CdZnTe crystal grown by the TGSG were investigated by PAL, which was based on the potential energy distribution and probability density of the positron of Positron in the crystal. The results showed that Cd vacancies had an increasing trend when the crystal ingot grew from initial growing region to stable growing region, while the content of Cd vacancies had a decreasing trend along the radial direction of the crystal (from center to edge). The lifetime of positron free state annihilation in CdZnTe crystal is about 216ps.

5. Acknowledgments

This work is supported by National Nature Science Foundation(No.11275122), Science and Technology Commission of Shanghai (No.11530500200) and Innovation Program of Shanghai Municipal Education Commission (No.12ZZ096). Thanks to the help from School of Physical Sciences ,University of Science and Technology of China.

References

- [1] Shin Hwa-Yuh , Sun Cherng-Yuan 1998 *J. Cryst. Growth*.**186** 67-78.
- [2] Limousin O 2003 *Nucl. Instrument. Methods Phys. Res.A* **504** 24-37.
- [3] Czock K.H, Arlt R 2001 *Nucl. Instrument. Methods Phys. Res.A* **458** 175-182
- [4] Turjanska L, Hoschl P, Belas E, Grill R, Franc J, Moravec P 2001 *Nucl. Instrument. Methods Phys. Res.A* **458** 90-95
- [5] Sang Wenbin, Qian Yongbiao, Shi Weiming 2000 *Journal of Crystal Growth*.**214/215** 30-34.
- [6] Krause-Rehberg R, Leipner H.S 1999 *Positron Annihilation in Semiconductors, Springer, Berlin*.
- [7] Dlubek G 1986 *J.Phys.C:Solide State Phys.***19** 331 344.
- [8] Gely Sykes C 1991 *Solid State Commun.*80:79.
- [9] Hautojarvi P 1995 *Mater Sci Forum*.**47** 175~ 178.
- [10] Vydyanath H.R. and Ellsworth J 1999 *J.Mater .Sci Lett.* **18** 695-697.
- [11] Vydyanath H.R, Ellsworth J. A, Fisher R. F 1993 *J. Electron. Mater.***29** 1067-1071.