Letter

# Lattice thermal expansion of $CdTe_{0.9}Se_{0.1}$ solid solution

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## Abstract

A lattice thermal expansion study of cubic $CdTe_{0.9}Se_{0.1}$ solid solution was carried out by high temperature X-ray powder diffraction technique (HTXRD) from room temperature to 773 K. An analytical least squares method for precise determination of the lattice constant for cubic crystals using a standard reference material as an external standard $2\theta$-calibrant was used in this investigation. The best estimated value of the lattice constant ($a$) for $CdTe_{0.9}Se_{0.1}$ was determined to be 6.441 (2) Å at 298 K. This value gradually increased to 6.457 (2) Å at 773 K. A similar trend was observed in the unit cell volume, which increased from 267.2(2) $Å^3$ to 269.3(2) $Å^3$ as the temperature changed from RT to 773 K. The thermal expansion coefficient was found to be $3.91 \times 10^{-6}\,K^{-1}$ at 298 K and continuously increased to $9.73 \times 10^{-6}\,K^{-1}$ at 773 K.
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## 1. Introduction

Alloys of II–VI compounds have attracted the attention as opto-electronic materials. The energy gap and electrical properties of these alloys vary with the compositions of the constituent compounds, which means that a semiconductor with specific properties can be prepared of these compounds [1–2]. This property would widen the scope of the applications, which cannot be achieved otherwise with a simple compound semiconductor. CdTe and CdSe are in the family of II–VI compounds, the former has cubic zincblende structure and the latter wurtzite structure. However, from structural point view $CdTe_{0.9}Se_{0.1}$ solid solution has different lattice parameter from both constituent compounds [3–4]. Studies of the thermal properties of this solid solution are important from the side of both fundamental physics and applications. In particular, the estimation of the coefficient of thermal expansion would be a valuable piece of information. For example, the normalization of the value of the lattice constant

to a specific temperature either for comparison with other workers or for application purposes requires knowledge of the thermal expansion coefficient of the material. To the best of our knowledge, no information is available in the open literature on the high-temperature thermal expansion characteristics of $CdTe_{0.9}Se_{0.1}$ solid solution. Therefore, the present study is aimed to estimate the thermal expansion characteristics by measuring accurately the lattice parameter variation as a function of temperature by high temperature X-ray powder diffraction technique (HTXRD) in the temperature range 298–773 K.

## 2. Experimental method

A powder sample of $CdTe_{0.9}Se_{0.1}$ solid solution was prepared by a solid state reaction method. The starting materials CdTe (purity 99.999%) and CdSe (purity 99.999%) were mixed in the required mole ratios and then placed into a silica tube evacuated to $6 \times 10^{-6}$ Torr. The silica tube was heated at $1323 \pm 5$ K for 5 h and was then furnace cooled to room temperature with an average cooling rate of 69 K/h

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to ensure homogeneity of the synthesized solid solution. The obtained compound was then ground and sieved to a size of 38 μm. The measurements were performed using a Shimadzu X-ray powder diffractometer (model XRD-7000) equipped with a vacuum heating stage (HA-1001). The diffraction studies were performed using Cu Kα radiation with θ–2θ geometery, crystal monochromator, divergence slit 1°, receiving slit 0.3 mm and proportional detector. The working conditions were 40 KV and 30 mA for the X-ray tube, scan speed 0.02°/s, a counting time of 6 s per step and angular range from 10° to 60° (2θ). The heating unit consist of a special sample heating furnace with an alumina ($Al_2O_3$) sample holder, temperature controller to an accuracy of about ±5 K and Pt–Rh thermocouple to monitor the temperature of the sample during the measurements. An average vacuum level of about $10^{-3}$ mbar was maintained throughout the measurements using rotary pump. Differential thermal analysis (DTA-Shimadzu 50) technique was conducted to test the thermal stability of the sample in the temperature range 300–1200 K with a heating rate of 10 K/min in a flowing nitrogen atmosphere.

## 3. Results and discussion

The dependence of the thermal expansion coefficient $\alpha$ on the lattice constant ($a$) is obvious from the relation $\alpha = (1/a_T)(da_T/dT)$. Therefore accurate measurements of the lattice constants result in good estimation of $\alpha$. However, in X-ray powder diffractometry the measured lattice constants are not accurate and suffer from both systematic aberrations and statistical errors [5]. The most important sources of systematic errors arise from the sample and instrument. Sample dependent errors are caused by the displacement of the specimen surface from the goniometer axis and from the absorption of X-rays in the specimen, while instrumental errors can be caused by misalignment and miscalibration of the instrument. The external standard method could correct for instrumental errors, but could not eliminate sample dependent systematic errors and random errors. Analytical least squares method for X-ray diffractometry was used in this study to correct the measured lattice constants for sample dependent errors and random errors [6–8]. The reference material used as external standard was silicon SRM 640c, certified for X-ray powder diffraction. The certified lattice constant of the standard was 5.4311946 ± 0.0000092 Å, at 295.5 K [9]. Knowing the thermal expansion coefficient of silicon, $2.76 \times 10^{-6}$ K$^{-1}$ [10], the constant was normalized to room temperature and the expected $2\theta_{calc}$ for silicon was then calculated. X-ray diffraction pattern was recorded from the standard at room temperature (Fig. 1) from which an external calibration curve was plotted between $\Delta 2\theta$ ($\Delta 2\theta = 2\theta_{calc} - 2\theta_{obs}$) and $2\theta_{obs}$. The correction values $\Delta 2\theta$ varied between −0.0001 and +0.0112 for the different peaks. The polynomial equation for the least squares fitted curve was obtained for the fourth degree (Fig. 1). This equation was then used to correct the $2\theta_{obs}$ values for the X-ray patterns of CdTe$_{0.9}$Se$_{0.1}$ solid solution. In order to correct
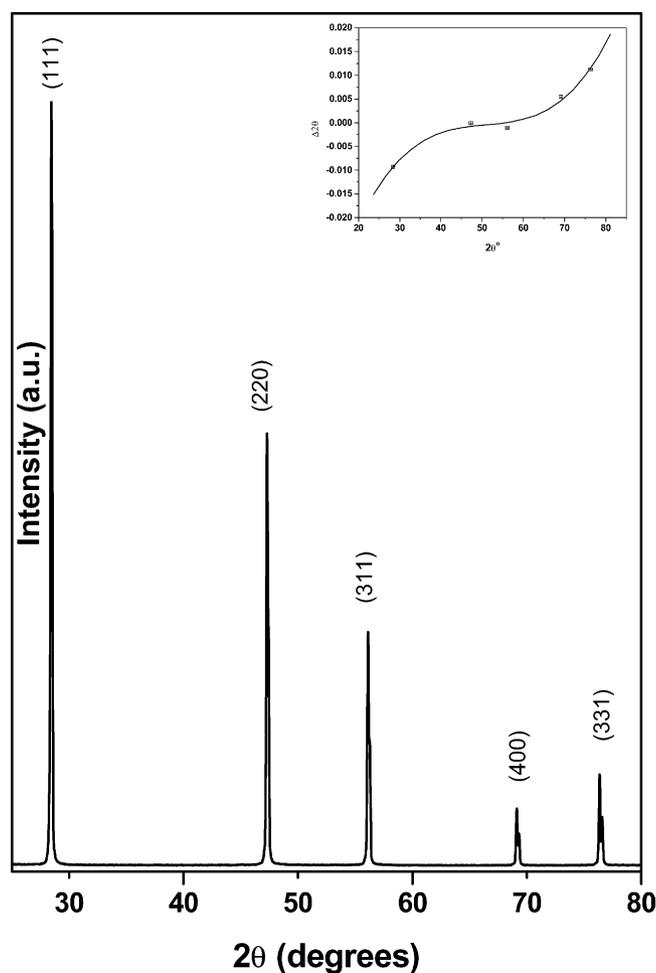


Fig. 1. X-ray diffractogram of silicon standard SRM 640c. The inset shows the calibration curve obtained from X-ray data of the silicon SRM 640c.

for all aberrations included in the peak positions, the use of external calibration method must be followed by the application of the analytical correcting method to the externally calibrated $2\theta$ values. The best estimates of the lattice constant for CdTe$_{0.9}$Se$_{0.1}$ at 298 K was found as $a = 6.441(2)$ Å, which is relatively close to our published value as $a = 6.4392(4)$ Å at 294 K [3] and can be considered as a refinement to the value of 6.4384 Å reported earlier[11]. Differential thermal analysis scans were made on the sample between 300 and 1200 K prior to X-ray measurements at elevated temperatures to examine the thermal stability of the sample. From the DTA result no significant thermal events can be observed at $T <$ 800 K, indicating that the sample is thermally stable in the investigated temperature range.

X-ray diffractograms were recorded from the CdTe$_{0.9}$Se$_{0.1}$ solid solution between 298 and 773 K. The XRD peaks present at room temperature are preserved up to 773 K except some extra traces refer to the alumina sample holder ($Al_2O_3$) [12]. The observed $2\theta_{obs}$ values for each pattern at the temperature of the measurement from the reflections {(111), (220), (311)} were then corrected for instrumental errors using the polynomial equation obtained
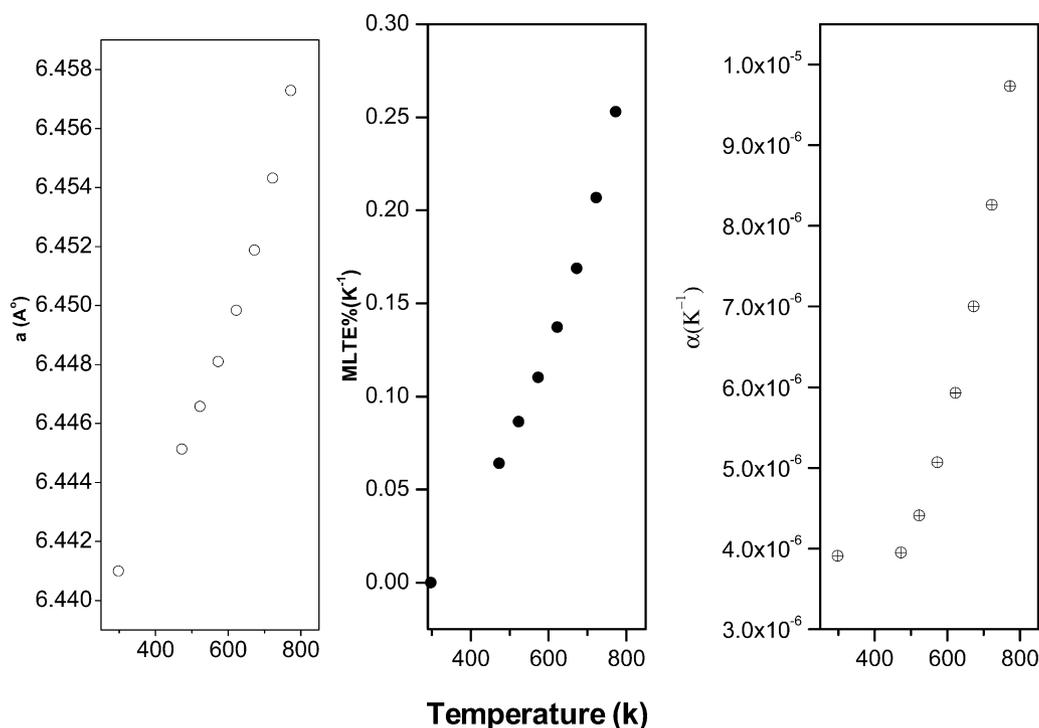
Fig. 2. Temperature dependencies of the lattice constant ($a$), mean linear thermal expansion (MLTE) and thermal expansion coefficient $\alpha$ of $CdTe_{0.9}Se_{0.1}$ solid solution.

from the calibrating standard SRM 640c. These corrected peaks positions were then analytically treated to give the best estimate of the lattice constants as a function of temperature.

The temperature dependence of the lattice constant for $CdTe_{0.9}Se_{0.1}$ sample is plotted in Fig. 2. The lattice constant increased from 6.441(2) Å at 298 K to 6.457 Å at 773 K. The percentage of the mean linear thermal expansion (defined as MLTE (%) = 100 $x$ $\{(a_T - a_{298})/a_{298})\}$) is graphically illustrated as a function of temperature in Fig. 2. For calculating the thermal expansion coefficient $\alpha$, the lattice constant (Å) variation with temperature (K) is fitted to a third degree polynomial given as:

$$a(\text{Å}) = 6.4293 + (6.14 \times 10^{-5}T) - (9.94 \times 10^{-8}T^2)$$
$$+ (8.65 \times 10^{-11}T^3)$$

Once the lattice constant is known as a function of temperature, it is then possible to estimate the thermal expansion coefficient ($\alpha = (1/a_T)\,(da_T/dT)$) as a function of temperature ($T$). Nonlinear dependence of the thermal expansion coefficient ($\alpha$) can be observed in Fig. 2 over the entire range of temperature. The estimated value of $\alpha$ was found to be 3.92 $\times 10^{-6}$ K$^{-1}$ at 298 K, which lies between the $\alpha$ values for the constituent compounds CdTe as 5 $\times 10^{-6}$ K$^{-1}$ and CdSe as $\alpha_a = 2.45 \times 10^{-6}$ K$^{-1}$, $\alpha_c = 4.4 \times 10^{-6}$ K$^{-1}$ at 300 K [13].

## 4. Conclusion

The thermal expansion characteristics of $CdTe_{0.9}Se_{0.1}$ solid solution have been investigated by measuring accurately

the temperature variation of lattice constant in the temperature range 298–773 K. Throughout this temperature range the sample seems to be stable and no phase transformation was observed. Continuous changes in the lattice constant and unit cell volume with temperature indicate the expansion of the unit cell. Estimated value of the thermal expansion coefficient of $CdTe_{0.9}Se_{0.1}$ at 298 K is different from both values of the constituent compounds and is found to be 3.92 $\times 10^{-6}$ K$^{-1}$.

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