

Letter

# Lattice thermal expansion of CdTe<sub>0.9</sub>Se<sub>0.1</sub> solid solution

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## Abstract

A lattice thermal expansion study of cubic CdTe<sub>0.9</sub>Se<sub>0.1</sub> 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<sub>0.9</sub>Se<sub>0.1</sub> 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<sup>3</sup> to 269.3(2) Å<sup>3</sup> as the temperature changed from RT to 773 K. The thermal expansion coefficient was found to be  $3.91 \times 10^{-6} \text{ K}^{-1}$  at 298 K and continuously increased to  $9.73 \times 10^{-6} \text{ K}^{-1}$  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<sub>0.9</sub>Se<sub>0.1</sub> 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<sub>0.9</sub>Se<sub>0.1</sub> 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<sub>0.9</sub>Se<sub>0.1</sub> 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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