Semiconductors, 2022, Vol. 56, No. 14

Thermal expansion of $Pb_{1-x}Cd_xTe$ crystals

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Received July 14, 2021
Revised August 3, 2021
Accepted August 3, 2021

The values of the lattice period and the linear coefficient of thermal expansion (α) of $Pb_{1-x}Cd_xTe$ solid solutions are determined depending on the cadmium content and temperature using high-temperature X-ray diffractometry. An increase in the concentration of cadmium in $Pb_{1-x}Cd_xTe$ in the range $x = 0.02-0.08$ leads to a significant increase in the linear coefficient of thermal expansion. A change in temperature range $T = 293-673$ K leads to decrease in the linear coefficient of thermal expansion. Besides, an increase in temperature does not affect the value α of the undoped PbTe in the indicated temperature range.

Keywords: lead telluride, cadmium, solid solutions, lattice period, linear coefficient of thermal expansion.

DOI: 10.21883/SC.2022.14.53865.9715

1. Introduction

Solid solutions $Pb_{1-x}Cd_xTe$ feature fine thermoelectric properties, since their high (and almost constant) thermoelectric coefficient combined with a constant electric conductivity within a fairly wide range of compositions, $x = 0.02-0.08$, provide an opportunity to synthesize crystals with specific properties on a reproducible basis and use them as highly efficient thermoelectric materials [1].

In the present study, high-temperature X-ray diffraction analysis is used to examine the dependence of the lattice period and the linear coefficient of thermal expansion on temperature and cadmium concentration in crystals of $Pb_{1-x}Cd_xTe$ solid solutions.

The obtained results may prove useful in choosing the interconnect materials for thermoelectric generators based on $Pb_{1-x}Cd_xTe$.

2. Experimental procedure

The synthesis and growth of $Pb_{1-x}Cd_xTe$ crystals were performed according to the procedure outlined in [2] with the use of high-purity Sigma-Aldrich materials: metallic lead (99.9995%), metallic cadmium (99.999%), and elementary tellurium (99.999%).

The PbTe crystal lattice structure is preserved in $Pb_{1-x}Cd_xTe$ solid solutions [3]. An ARL X'TRA diffractometer fitted with a heater and a vacuum chamber was used to study the composition and temperature dependence of the lattice period of $Pb_{1-x}Cd_xTe$. Filtered CuK_α radiation with Bragg–Brentano focusing was applied in these experiments. Measurements were performed with a 2Θ pitch of 0.01°. Powdered samples for X-ray analysis were prepared from the synthesized $Pb_{1-x}Cd_xTe$ crystals. Interplanar distances were calculated based on the centroids of reflections, and the lattice period was calculated using the Nelson–Riley extrapolation function [4] with account for all reflections in the diffraction pattern. The random error of the lattice parameter was estimated as the error of linear approximation of the extrapolation function. In addition, the correction for expansion of the sample holder under heating was introduced.

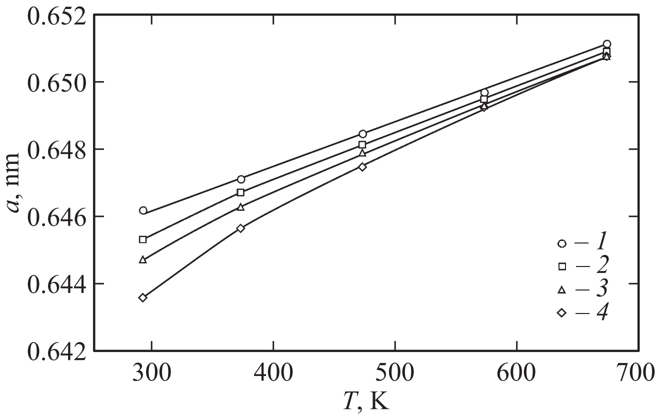
Linear coefficient of thermal expansion α was determined as the variation of period $a_T - a_0$ of a cubic lattice within the corresponding temperature interval $T - T_0$ [5]:

$$\alpha = \frac{1}{a_0} \cdot \frac{a_T - a_0}{T - T_0}. \qquad (1)$$

3. Experimental results

According to the data from [2,6], the solubility of cadmium in $Pb_{1-x}Cd_xTe$ at the annealing temperature used in the present work (943 K) with subsequent quenching corresponds to $x = 0.08$. In the present study, the lattice period of $Pb_{1-x}Cd_xTe$ solid solutions with cadmium concentrations $x = 0$, 0.02, 0.04, 0.08 was examined at temperatures $T = 293$, 373, 473, 573, 673 K. The appreciable volatility of components of these materials (especially cadmium) limits their application at higher temperatures.

Temperature dependences of the lattice period of $Pb_{1-x}Cd_xTe$ solid solutions of various compositions are presented in the figure. The error of determination of the lattice period was within $\pm 5 \cdot 10^{-5}$ nm. It can be seen that the lattice period of $Pb_{1-x}Cd_xTe$ solid solutions increases with temperature and decreases as the cadmium concentration grows. Affected by these two opposing trends, the lattice periods of solid solutions with high cadmium concentrations remain almost constant at high temperatures and are close in magnitude to the lattice period of undoped PbTe.



Temperature dependence of the lattice period of $Pb_{1-x}Cd_xTe$ solid solutions with different concentrations of cadmium, x: *1* — 0, *2* — 0.02, *3* — 0.04, *4* — 0.08.

Interestingly, the temperature dependence of the lattice period of undoped PbTe is linear; as the cadmium concentration grows, the dependence becomes more and more non-linear (especially at temperatures of 293−373 K).

The values of linear coefficient of thermal expansion of $Pb_{1-x}Cd_xTe$ solid solutions, which were calculated for various compositions and temperatures using formula (1), are listed in the table. The lattice period at temperature $T_0 = 293$ K was used as the initial linear size a_0.

Linear coefficient of thermal expansion of $Pb_{1-x}Cd_xTe$ solid solutions for various compositions and temperatures ($\alpha \cdot 10^6\,K^{-1}$)

T, K	Cadmium concentration, x			
	0	0.02	0.04	0.08
373	20.05	26.56	30.14	40.05
473		24.18	27.21	33.38
573		22.94	25.18	31.35
673		22.67	24.55	29.19

Since the lattice period of undoped PbTe increases almost linearly in the studied temperature range, a constant linear coefficient of thermal expansion corresponds to it. When the concentration of cadmium in $Pb_{1-x}Cd_xTe$ grows, the linear coefficient of thermal expansion increases markedly; heating has the opposite effect.

4. Conclusion

Undoped PbTe has a constant linear coefficient of thermal expansion at temperatures of 293−673 K. When the concentration of cadmium in $Pb_{1-x}Cd_xTe$ grows, the linear coefficient of thermal expansion increases; heating, however, has the opposite effect.

Acknowledgments

The author would like to thank his colleague S.V. Kannykin at the common use center of the Voronezh State University for performing the measurements with an ARL X'TRA-ray diffractometer.

Conflict of interest

The author declares that he has no conflict of interest.

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