Experimental and theoretical analysis of room temperature thermoelectric and thermal properties of PbTe-CdTe solid solution

M. Szot, K. Dybko, P. Pfeffer, A. Szczerbakow, L. Kowalczyk, P. Dziawa, T. Zayarnyuk, K. Piotrowski, M. U. Gutowska, A. Szewczyk, W. Zawadzki, T. Story

Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland

The relentless focus on the investigation of PbTe-CdTe semiconductor system originates from the expectation, that addition of Cd can improve widely known good thermoelectric properties of PbTe. Moreover, limited mutual solubility of both semiconductors favors this system in realization of the idea of phonon-glass electron-crystal material for thermoelectric applications in the form of PbTe-CdTe nanocomposite [1]. So far only polycrystalline $Pb_{1-x}Cd_xTe$ bulk samples with low Cd content $x \approx 0.01$ were studied [2]. In this paper we present the results of experimental and theoretical studies of thermoelectric properties of $Pb_{1-x}Cd_xTe$ crystals grown by self-selecting vapour growth method [3]. This growth technique allows to obtain the high quality monocrystalline $Pb_{1-x}Cd_xTe$ ternary semiconductor with Cd content up to $x \approx 0.11$. The investigated samples exhibit *p*-type conductivity for all Cd content studied, with the room temperature carriers concentration changing in the range from $p \approx 4\times10^{18}$ cm^{-3} to $p \approx 2\times10^{18} cm^{-3}$ with x increasing from 0.01 to 0.11. Increase of Cd content leads to an enhancement of *Seebeck* coefficient from $S \approx 220$ μV/K for $x \approx 0.01$ to 500 μV/K for $x \approx 0.1$. and for samples with high x observed thermopower is considerably improved with respect to the reference p-PbTe crystals (*Pisarenko* plot). This important experimental finding we analyze theoretically within the two-band ***k·p*** model, in which the increase of effective mass of light holes, resulting from experimentally confirmed increase of energy gap in $Pb_{1-x}Cd_xTe$ crystals, was taken into account. Further, the total thermal conductivity κ of investigated samples decreases from 2 $Wm^{-1}K^{-1}$ for reference PbTe to 0.9 $Wm^{-1}K^{-1}$ for $x = 0.09$ crystal. Since the electronic part of the thermal conductivity in the case of $Pb_{1-x}Cd_xTe$ is limited by relatively low conductivity, the observed decrease of κ is attributed to the enhanced phonon scattering on disorder within the unit cell of $Pb_{1-x}Cd_xTe$ crystal arising from the substitution of Pb ions by Cd. The observed thermal conductivity behavior of $Pb_{1-x}Cd_xTe$ crystal with increasing Cd content is well described based on Callaway approximation [4].

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