Inelastic Neutron Scattering Studies of Acoustic-Optical Phonon Coupling in (Pb,Cd)Te Solid Solution

Rafał Kuna [1], Katarzyna Gas [1], Patrick Baroni [2], Sylvain Petit [2], Roman Minikayev [1], Andrzej Szczerbakow [1] and Wojciech Szuszkiewicz [1]*

[1] *Institute of Physics, PAS, Al. Lotników 32/46, 02-668 Warszawa, Poland*
[2] *Laboratoire Léon Brillouin, CEA-CNRS, CE Saclay, 91191 Gif-sur-Yvette Cedex, France*

PbTe is one of the leading thermoelectric materials transforming heat into potentially useful electricity. The thermoelectric figure of merit, which describe the maximum efficiency of the conversion process, depends on both electrical and thermal conductivity. The efficient thermoelectric materials should demonstrate a low thermal conductivity and, in particular, the lattice contribution to it. The origin of the low PbTe lattice conductivity has been explained only very recently by a strong anharmonic coupling between the acoustic and optical phonon modes, demonstrated by inelastic neutron scattering measurements [1]. However, possible modification of suggested physical mechanism with an increasing composition of a PbTe-based solid solution remain unknown.

Recent successful growth of big, metastable (Pb,Cd)Te single crystals by self-selecting vapour transport in the Institute of Physics PAS [2,3] opened new experimental opportunities. The goal of present work was to investigate the phonon dispersion in (Pb,Cd)Te solid solutions containing about 5 at% and 9 at% of CdTe. The RT measurements were performed in LLB with the use of 2T1 spectrometer installed on the thermal source. In spite of high neutron absorption resulting from a presence of Cd in investigated bulk crystals and an additional phonon damping resulting from the alloy scattering it was possible to get some data and to determine TA, LA, and TO phonon dispersion along selected high-symmetry directions in the Brillouin zone. In order to complete our data the inelastic neutron scattering measurements were also performed for PbTe single crystal using G4.3 spectrometer, where the cold neutron beam is applied.

Our results demonstrate slight increase of TO modes frequencies with increasing CdTe content in (Pb,Cd)Te solid solution. In the case of LA phonon mode dispersion along [001] direction small shift of this mode maximum and significant evolution of its FWHM in the vicinity of Q=(0 0 0.8) is observed. Present data suggest that LO phonon mode frequency at the Γ point of the Brillouin zone noticeable increases with the CdTe content. Possible influence of observed modifications of the lattice dynamics in solid solution on thermoelectric efficiency of the material under studies is analyzed and discussed.

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* Corresponding author. E-mail address: szusz@ifpan.edu.pl.