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Inelastic X-ray scattering as a tool to study the phonon dispersion in PbTe and (Pb,Cd)Te solid solution

R. Minikayev[1]*, R. Kuna[1], M. Trzyna[2], A. Szczerbakow[1], K. Gas[1,3], J. Łażewski[4], A. Bosak[5] and W. Szuszkiewicz[2,1]

[1]*Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*
[2]*Faculty of Mathematics and Natural Sciences, University of Rzeszów, ul. S. Pigonia 1, 35-310 Rzeszów, Poland*
[3]*Institute of Experimental Physics, University of Wrocław, pl. M. Borna 9, 50-204 Wrocław, Poland*
[4]*Institute of Nuclear Physics PAS, ul. Radzikowskiego 152, 31-342 Kraków, Poland*
[5]*ESRF - The European Synchrotron, 71 avenue des Martyrs, 38000 Grenoble, France*

Keywords: synchrotron radiation, thermoelectric materials inelastic X-ray scattering

*e-mail: minik@ifpan.edu.pl

Thermoelectric materials are of great interest for the energy applications because they can transform heat into electricity [1]. An efficient thermoelectric material should exhibit the same time a low heat conductivity and a high electric conductivity. A good knowledge of the lattice dynamics is essential in order to understand both heat and electron transport in such material.

Lead telluride (PbTe) is well known thermoelectric semiconductor (SC) crystallizing in the rock-salt (RS) structure, cadmium telluride (CdTe) is the SC exhibiting the sphalerite structure [2]. The difference in PbTe and CdTe crystal symmetry was in the past the principal reason of many problems in a growth of the (Pb,Cd)Te solid solution. Recent successful growth of big (with a volume exceeding 1 cm^3), metastable (Pb,Cd)Te single crystals with the RS structure obtained by Self-Selecting Vapour Growth (SSVG) method at the Institute of Physics PAS [3] changed this situation. In the present work the bulk, single PbTe crystal and the (Pb,Cd)Te solid solution with 2% of CdTe grown by the SSVG were used to investigate the phonon dispersion.

Primary parameters describing collective atom motion in the crystal lattice are momentum transfer (Q) and energies (E), that could be obtained via experimental method, such as the inelastic neutron scattering (INS). In the middle of 70's an idea has appeared to investigate the lattice dynamics using an inelastic X-ray scattering (IXS) [4] and it was the experimental technique applied in the present work. The ID28 beamline in ESRF equipped with the IXS spectrometer enabling one to study phonon dispersion in condensed matter was used for this purpose. The high energy of incident photons (E = 17.8 keV) leads to a possibility to investigate phonons for every momentum in Brillouin zone (BZ). The phonon dispersion in the PbTe and (Pb,Cd)Te solid solution was investigated along Γ-X [100] and Γ-K [110] high-symmetry directions in the BZ. We determined the phonon dispersion for all modes along the [100] direction and for two phonon branches only (TO, TA) along the [110] direction both in PbTe and (Pb,Cd)Te. Due to the extremely high energy resolution of scattered photons ($\Delta E/E = 10^{-7}$) the accuracy of relevant phonon dispersion was comparable to that corresponding to the INS measurements in spite of low energy of phonons in the PbTe-based crystals. The IXS results confirmed the INS data obtained previously for PbTe and show an increase of the full-width at half-maximum (FWHM) value for TO phonon mode close to the BZ center along Γ-X and Γ-K directions.

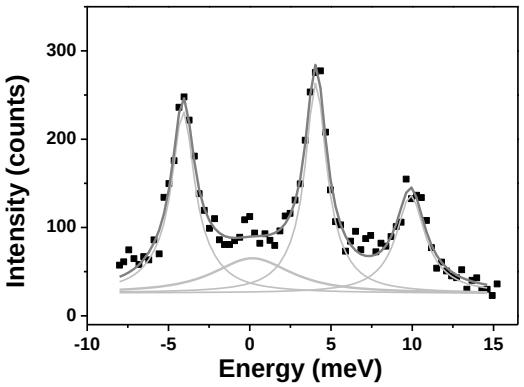

Figure 1. Part of the IXS spectrum taken for PbTe for Q = (0,0,0.7). Points – experimental data, solid lines – result of the fit. Two high-intensity structures correspond to the absorption and the excitation of LA phonon, third structure is due to the excitation of the LO phonon.

Acknowledgments: This work was partially supported by the research grant (UMO-2014/13/B/ST3/04393) from National Science Center (Poland), by the European Synchrotron Radiation Facility (ESRF), Grenoble (France) and by the EAgLE project (Project Number: 316014) from EU.

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