Inelastic X-ray Scattering Studies of the Phonon Dispersion in PbTe and (Pb,Cd)Te Solid Solution

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Thermoelectric materials are of great interest for energy applications transforming heat into electricity. Lead telluride PbTe is a well known thermoelectric semiconductor (SC) with rock salt structure, while cadmium telluride CdTe is of sphalerite structure. The difference in the PbTe and CdTe crystal structure types strongly limits the composition range of the (Pb,Cd)Te solid solution. Investigation and interpretation of the lattice dynamics is essential in order to understand heat and electron transport in SCs. Primary parameters describing collective atom motion in the lattice are momentum transfer (Q) and energy (E), that could be measured by neutron spectroscopy (inelastic neutron scattering - INS). In the 70's an idea has emerged to investigate lattice dynamics using inelastic X-ray scattering (IXS). Recent successful growth of relatively big (~1 cm^3), metastable (Pb,Cd)Te single crystals with the rock salt structure obtained by self-selecting vapour growth (SSVG) method at the Institute of Physics PAS [1,2] made it possible to investigate their lattice dynamics by the INS technique. In the present work bulk crystals of pure PbTe, as well as of (Pb,Cd)Te solid solution with 2% of CdTe, were used to determine the phonon dispersion by the IXS and to check our selected results obtained by the INS method.

The ID28 beamline in ESRF used for the measurements reported here is equipped with a typical IXS spectrometer for studying phonon dispersion in the condensed matter. High energy of interacting photons (E = 18 keV) leads to the possibility of investigating phonons for every momentum in the Brillouin zone (BZ), and an extremely high energy resolution ($\Delta E/E = 10^{-7}$) of scattered photons was achieved. Almost complete phonon dispersion for PbTe and (Pb,Cd)Te solid solution was determined in the BZ along Γ-X ([100]) direction, we have also observed phonon dispersion for two branches (TO, TA) along Γ-K ([110]) direction in both PbTe and (Pb,Cd)Te as well. The IXS results confirm our INS data and show, e.g., an increase of the FWHM value for TO phonon mode close to the BZ center along Γ-X and Γ-K directions. However, some of our results do not agree with selected findings reported previously in [3].

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