Temperature Dependence of Phonon Dispersion and TO-Phonon Anharmonicity in PbTe and (Pb,Cd)Te Solid Solution

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PbTe and selected solid solutions obtained on the basis of this IV-VI compound are known as very efficient thermoelectric materials transforming heat into potentially useful electricity. The origin of the low PbTe lattice thermal conductivity has been explained recently in *Nature Materials* [1] by a strong anharmonic coupling between the optic and the acoustic phonon modes, demonstrated by inelastic neutron scattering (INS) measurements at room temperature, using the time-of-flight technique. Another explanation of the low PbTe lattice thermal conductivity has been presented a few years ago [2, 3]. The authors of these papers observed a supplementary phonon mode in the Brillouin zone center and in its vicinity, and suggested a presence of lattice local symmetry lowering as possible origin of this effect.

The aim of present work was to investigate details of the phonon dispersion in PbTe and (Pb,Cd)Te solid solution as a function of temperature and to analyze the strong TO–phonon anharmonicity, reported previously in the literature. The INS measurements with the use of triple-axis spectrometer were chosen as the experimental technique for that purpose.

The high quality, single (Pb,Cd)Te crystals containing 0.6% and 1.9% of CdTe and pure PbTe were prepared by self-selecting vapour growth technique (SSVG) [4] and characterized at the Institute of Physics PAS by XRD. All investigated samples have the *fcc* crystal structure of the NaCl type. The INS measurements were performed at LLB with the use of 2T1 triple-axis spectrometer installed at the thermal neutron source. The phonon dispersion and phonon damping along the [001] and [011] directions were determined at a few temperatures from 3.5 K to 295 K. In order to get an information on a strong TO-phonon mode anharmonicity, the frequency and damping of this mode were investigated at the Γ point of Brillouin zone at several temperatures. The softening of TO phonon mode with decreasing temperature was observed at this point for both PbTe and (Pb,Cd)Te solid solution. On the contrary, in all investigated samples the TO phonon frequency remains almost fixed at Brillouin zone boundary. The temperature dependences of other phonon branches are also shown and discussed.

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