Neutron scattering studies of phonon dispersion in (Pb,Cd)Te solid solution

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PbTe is one of the leading thermoelectric materials transforming heat into potentially useful electricity. The origin of the low PbTe lattice thermal conductivity has been explained only very 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 using the time-of-flight technique. In particular, according to the authors of paper [2] this coupling leads to an avoided-crossing behaviour in the dispersion of TO and LA phonon modes accompanied by an anomalous modification of both dispersion and damping of phonon branches. Another explanation of the low PbTe lattice thermal conductivity has been presented a few years ago in two papers published in *Science* and *Phys. Rev. B* ([3] and [4], respectively). The authors of these papers observed a supplementary phonon mode in the Brillouin zone centre and in its vicinity, and suggested a presence of lattice local symmetry lowering as possible origin of this effect.

The goal of present project was to investigate the phonon dispersion in PbTe and (Pb,Cd)Te solid solution and to check these findings by both the precise, 'classical' neutron triple-axis spectrometry and by *ab initio* calculations based on density functional theory (VASP package) and the direct force constants method (PHONON package).

The highest quality (Pb,Cd)Te single crystals with the rocksalt structure containing up to 9% of CdTe in the solid solution were prepared by self-selecting vapour growth technique (SSVG) [4] and characterized at the Institute of Physics PAS. The INS measurements were performed at LLB with the use of 1T and G4.3 triple-axis spectrometers taking advantage of thermal and cold neutrons, respectively. The phonon dispersion and phonon damping along the [001] and [011] directions were determined at room temperature. In order to get an information on a strong TO phonon mode anharmonicity, suggested in the literature, the frequency and damping of this mode were also obtained at low temperatures at several points scattered along the [001] direction. In the theoretical calculations anharmonic effects were derived from dependence of phonon frequencies on normal mode amplitude. The high precision data obtained for PbTe will be compared with the literature ([1-3]) results, possible reasons of observed differences will be discussed in detail.

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