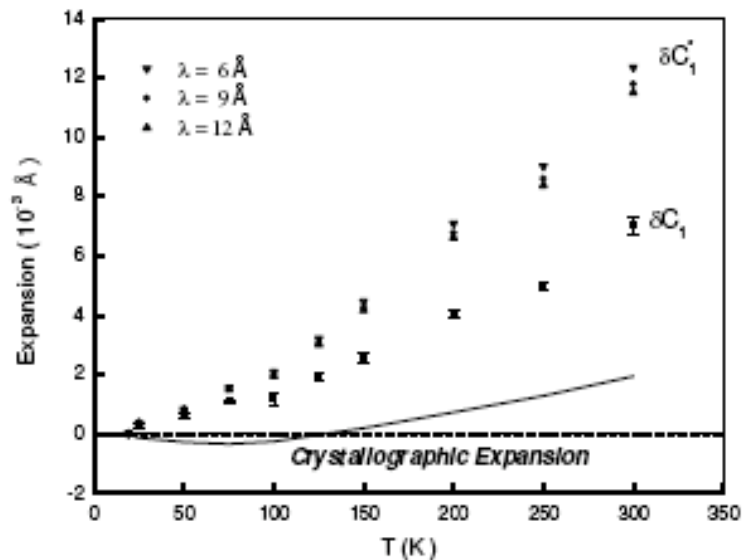


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"Local lattice dynamics and negative thermal expansion in zinc-blende semiconductors.
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The research program concerned the measurement of the thermal expansion of the nearest-neighbours bonds in CdTe and HgTe and of the corresponding MSRDs. Aim of the experiment was to find a correlation between negative thermal expansion (NTE) properties and quantities measured by EXAFS in tetrahedrally coordinated semiconductors. The properties of CdTe and HgTe are intermediate between those of Ge and CuCl, on which EXAFS measurements had been previously performed. Un unusual sequence of beamline technical problems reduced the useful shifts to four. As a consequence, EXAFS could be measured only at the K edge of Cd in CdTe, from 19 to 300 K. The quality of the spectra was anyway good, and the first shell analysis gave significant results.

The bond thermal expansion, measured by the first cumulant δC_1^* of the real distribution of distances, is positive in the full explored range (see figure, where also the crystallographic expansion and the δC_1 of the effective distribution are shown). A positive bond expansion has been found up to now for all NTE crystals studied by EXAFS.



The difference between the thermal expansions measured by EXAFS and by diffraction has been exploited to evaluate the perpendicular MSR, and the ratio perpendicular to parallel MSR, which measures the anisotropy of relative vibrations.

The values of the force constants best-fitting both parallel and perpendicular MSR, and of the anisotropy ratio are intermediate between the values found for Ge and CuCl, confirming that a relation exists between NTE properties and quantities measured by EXAFS. Further work is in progress to analyze the outer coordination shells.

The resolution and accuracy of bond thermal expansion obtained in this experiment suggest that, by measuring interatomic distances at much shorter temperature steps, one could perform a derivative with respect to temperature, and evaluate the coefficient of bond thermal expansion.