

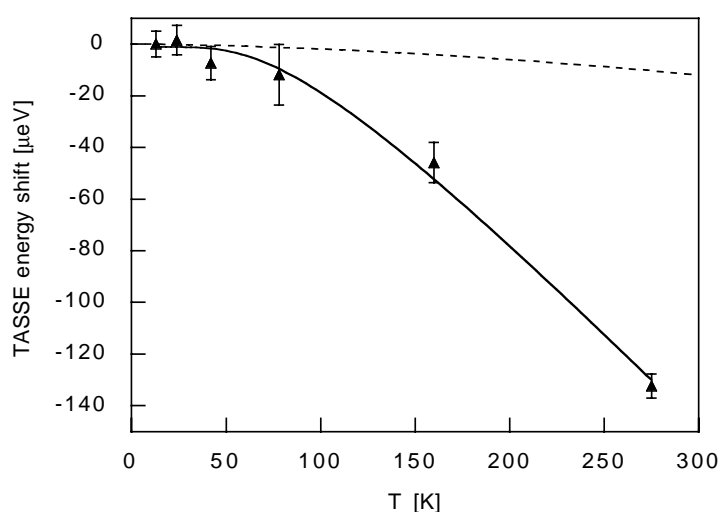
Neutron TAS spin-echo – a handle to anharmonic effects in lattice dynamics.

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The access to experimental information on weak anharmonic effects in lattice dynamics, such as thermal variation of phonon frequencies and their natural line-widths in crystals far from structural phase transitions, is a long-standing problem. While optical spectroscopy can provide such information on optically active phonons at the Brillouin zone center, the extraction of similar information from neutron scattering data for phonons at an arbitrary position in the Brillouin zone is almost impossible. Much improvement to this situation is expected from the enhancement of the energy resolution of the classical three-axis spectrometers (TAS) by combination with the neutron spin-echo technique, used so far mainly for quasi-elastic scattering studies.

The TASSE option of the IN20 spectrometer at the ILL is a prototype of such a set-up, employing two optimized field shape superconducting coils, which provide a field integral of about 1 Tm. The maximum Fourier time of 3.2 ns for neutrons with $k = 2.661 \text{ \AA}^{-1}$ permits to reach a quasi-elastic resolution of 10 neV [1]. Although at energy transfers comparable to the neutron energy, the optimum spin-echo condition cannot be met exactly, the deteriorated resolution is still sufficient to permit excitation studies with a relative resolution of 10^{-3} - 10^{-4} previously inaccessible to neutron TAS spectroscopy.



In the past two years several experiments have been carried out on IN20 to exploit these new possibilities, ranging from critical scattering studies [1] over excitations in superfluid helium [2] to phonon studies in group-IV semiconductors, whose anharmonic behaviour can be calculated by *ab initio* techniques. As an example of an inelastic study involving energy transfers of 10 meV, our figure displays the temperature variation of the frequency of a zone-boundary ‘transverse acoustic’ phonon in the [100] direction in germanium [3]. The present data match perfectly the previous high-temperature results of ref. [3] and confirm that in the whole temperature range the phonon frequency follows the prediction of Barron’s model (full line), based on the harmonic vibrational energy of the crystal, rather than to scale with the crystal volume variation as predicted by the simple quasiharmonic approach (dotted line).

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