ESRF	**Experiment title:** The phonon dispersion in zinc-blende Silicon Carbide	**Experiment number:** HS-1498
Beamline: ID28	**Date of experiment:** from: June 27th, 2001 to: July 10th, 2001	**Date of report:** February 1st, 2002
Shifts: 30	**Local contact(s):** M. Lorenzen, H. Requardt	*Received at ESRF:*

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Report:

With the advent of highly brilliant third generation synchrothron facilities, inelastic X-Ray scattering (IXS) has become an alternative technique to measure the phonon dispersion relations in single crystals with comparable or sometimes even better resolution than that achieved by inelastic neutron scattering (INS), the technique traditionally used in the past thirty years. Although it is mainly devoted to investigate the dynamics of liquids [1], the small size of the beam diameter makes IXS a unique technique for the investigation of lattice dynamics in single crystals that cannot be grown large enough for carrying out INS experiments. This is the case of some interesting semiconductors, as GaN and SiC where INS has not been employed because of the lack of sizeable crystals. For these compounds there is not enough information about the phonon properties which can lead to important effects e.g. in the thermal conductivity, although they have been investigated thoroughly because of their applications in optoelectronic devices.
In a previous experiment we performed IXS measurements at ESRF in diamond and GaN (project HS-1068), which yielded for the latter a good description of the silent B_1 modes, especially difficult to tackle with other techniques [2].

Here we report measurements by IXS of the phonon dispersion relations of zinc blende (3C) silicon carbide over the entire Brillouin zone. The energy of the incident radiation (17.794 keV) was defined by the silicon (999) Bragg reflection at the monochromator, yielding an instrumental energy resolution of ≈ 20 cm^{-1} and a momentum resolution of ≈ 0.28 cm^{-1}. With this configuration, phonon frequencies were determined to within ± 2 cm^{-1}. As a guide for the experiment to determine the optimal scattering geometries, we performed *ab-initio* calculations of the phonon dispersion based on density functional theory.

In Fig. 1 we display the measured data (solid circles) together with the calculated dispersion (solid lines), and Raman data [3] along the Γ–L direction (open diamonds) obtained from different polytypes using the backfolding technique. There is very good agreement between the IXS data and the *ab-initio* results, with deviations less than 3%. Eigenvector analysis of the IXS data allows the assignment of longitudinal and transverse character of the different phonon branches. This is specially important along the Γ–K–X direction, where e.g. the phonon frequencies measured for the transverse optic modes correspond to the lower branch, in agreement with the calculation.

In order to extract information about the differences in the phonon dispersion caused by the different stacking planes in several polytypes of SiC, we also performed some measurements by IXS on the hexagonal modification 4H-SiC. In Fig. 2 we show the IXS data for 3C-SiC along the Γ–L direction (open circles) together with those obtained for the 4H-SiC (open squares) and Raman data from other hexagonal and rombohedral polytypes, along the c-axis, backfolded onto the 3C-SiC dispersion. The open triangles correspond to INS data on 6H-SiC for the c-axis [4]. In spite of the different second nearest neighbor arrangement, there is a clear overlap between the data of all the polytypes. The dashed lines represent *ab-initio* calculations for the 4H modification.

In summary, the experiment reported here provides a valuable contribution to the vibrational properties of silicon carbide for the 3C and 4H crystal structures, yielding for the former the phonon dispersion over the entire Brillouin zone. It also validates the backfolding approximation used to estimate the phonon dispersion along the Γ–L direction by Raman data of different polytypes.

As a result of the measurements performed in the beamline ID28 at ESRF, we have submitted the following contribution:

Determination of the phonon dispersion of zinc blende (3C) Silicon Carbide by inelastic X-ray scattering, J. Serrano *et al.*, submitted to Appl. Phys. Lett. (January 18th, 2002).

Another paper describing more thoroughly the results for 4H-SiC is forthcoming.

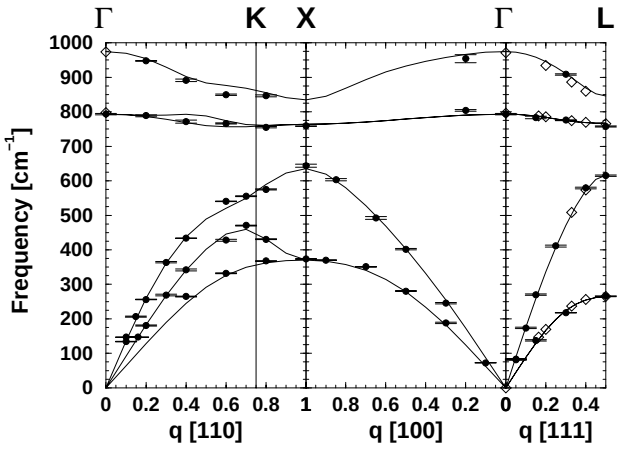

Fig. 1

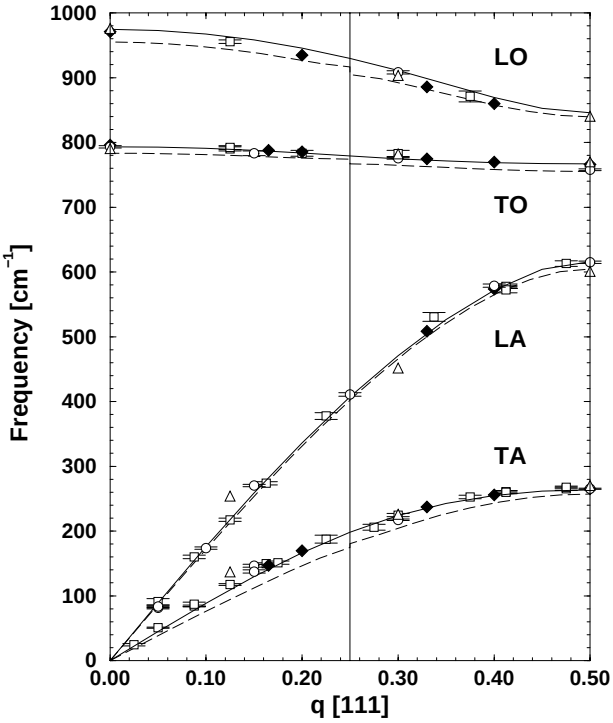

Fig. 2

References

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