ESRF	**Experiment title:** Investigation of the quasi-optical phonon branches in 4H-SiC	**Experiment number:** HS-2609
Beamline: ID28	**Date of experiment:** from: Nov. 26th, 2004 to: Dec. 7th, 2004	**Date of report:** February 18, 2005
Shifts: 21	**Local contact(s):** Alexey Bosak	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
Dieter Strauch (main proposer), Michael Malorny (1)
Bruno Dorner (*,3)
Wolfgang J. Choyke (*,2)
Michael Krisch, Jorge Serrano (*,4)
(1) Universität Regensburg, Regensburg, Germany
(2) University of Pittsburgh, Pittsburgh,U.S.A.
(3) Institute Laue Langevin, Grenoble, France
(4) European Synchrotron Radiation Facilities, Grenoble, France

Report:

Silicon carbide is a semiconducting material which has attracted much interest because of its applications for opto-electronic devices and its hardness and high thermal conductivity. It grows in a vast number of polytypes, the 4H modification having a band gap of 3.2 eV, suitable for emission in the blue-ultraviolet spectral region. The characterization of the lattice dynamics in this material allows us to understand physical properties such as the thermal conductivity, relevant for the development of electronic devices.

4H-SiC has an hexagonal crystal lattice with eight atoms per unit cell and 24 branches in the phonon dispersion relations. Although some of them are degenerate along certain high symmetry directions, the determination of the individual phonon frequencies and the discrimination of the phonon group symmetry can only be realized by a measurement strategy combining high resolution inelastic x-ray scattering experiments and reliable theoretical predictions for the phonon frequencies and relative intensities for different scattering geometries, the latter being available through an accurate calculation of phonon eigenvectors.

We have performed IXS measurements of the phonon dispersion relations of 4H-SiC at the beam line ID28. For this purpose, a single crystal of $5 \times 3 \times 0.2$ mm^3 with the surface oriented perpendicular to the $[11\bar{2}0]$ direction was employed.

The aims of this project were the measurement of the twelve quasi-optic phonon branches, which are distributed into two energy ranges: The eight transverse optic modes (TO) lie near each other in the 80–90 meV range, whereas the four longitudinal optic modes (LO) lie in the 100–120 meV range. The high energy resolution required to separate the different branches within these two ranges was achieved by using 17.794 keV x-rays obtained from the 999 reflection of a silicon monochromator at ID28. The energy and momentum resolution were 3 meV and 2.4 nm^{-1}, respectively. The IXS measurements were performed at 300 K, selecting between transmission and reflection scattering geometries depending on the required total momentum transfer $\mathbf{Q}$. The latter was chosen for a given phonon momentum $\mathbf{q}$ according to predictions made from *ab initio* calculations of the scattered intensities we had previously performed using density functional perturbation theory [1].

Frequencies and relative intensities, the latter also depending upon the eigenvectors, were carefully measured for TO and LO phonons along the Γ-K-M ([ξ ξ 0]), A-H-L ([ξ ξ 0.5]), and L-M ([0.5 0 ξ]) directions. The agreement between calculated and experimentally observed phonon frequencies is remarkable, as illustrated in Fig. 1, where we show the optic dispersion branches along the A-H-L direction. Similar agreement was obtained for the other investigated directions. The analysis of phonon eigenvectors is more involved and still in progress. However, first conclusions can be drafted from the success of the experiment. The predictions for the relative intensity among the different phonon peaks for both a given momentum transfer and among several scattering geometries agree qualitatively in all the cases with the observed intensities. This was an essential fact for the analysis of the mode symmetry and assignment of the phonons to the different branches. Simple selection rules were fulfilled by the calculations and observed in the experiment: The twelve optic phonon branches corresponding to the Γ-K-M direction can be divided into two groups of six phonons each, the first group observable at momentum transfers (ξ, ξ, l) with l odd and the second group allowed only for even values of l. This observation is also valid for the optic branches along the L-M direction as well as for their respective acoustic branches. Another example is the mirror symmetry of the atomic planes at $c/2$, which causes the phonon branches to be doubly degenerate in the $\langle \xi_1\ \xi_2\ 0.5 \rangle$ plane.

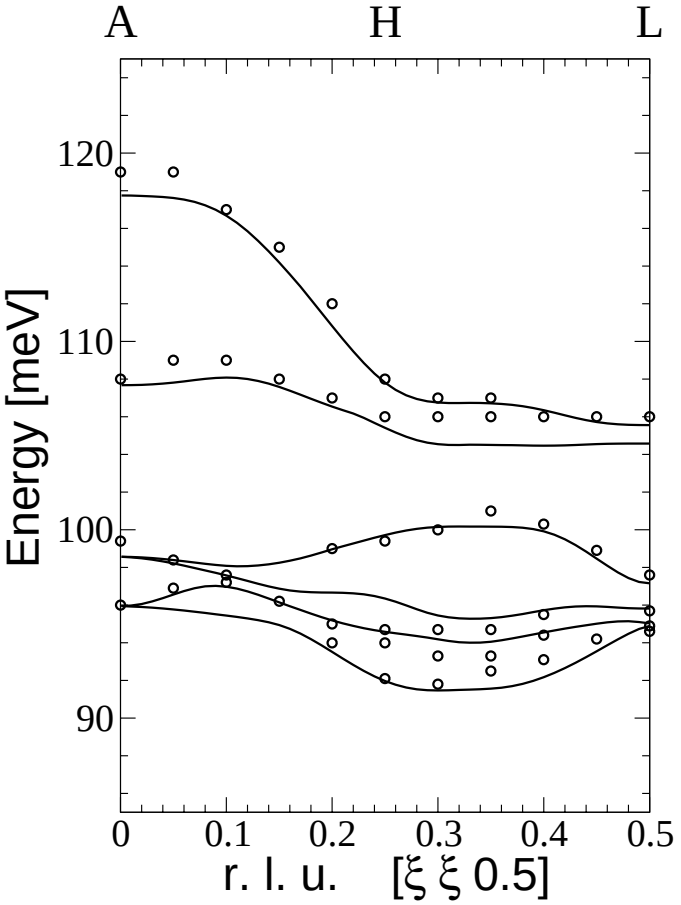
In summary, the experiment reported here provides valuable information of the lattice dynamics of 4H-SiC and contributes to the evaluation of the quality of first principles calculations of the phonon frequencies and eigenvectors. The optic phonon branches of the dispersion relations have been obtained and the relative intensities calculated for different scattering geometries agree at least qualitatively with the measured intensities. A further analysis of the eigenvectors is in progress and will be reported elsewhere. This experiment complements very nicely previous measurements performed with IXS at ID28 on SiC-4H and zinc blende (3C) SiC (see report for experiment HS-1498 and references [2,3]).

References

[1] First-principles computation of material properties : the ABINIT software project. X. Gonze *et al.*, Computational Materials Science 25, 478-492 (2002).

[2] Determination of the phonon dispersion of zinc blende (3C) silicon carbide by inelastic x-ray scattering, J. Serrano *et al.*, Appl. Phys. Lett. 80, 4360 (2002).

[3] Lattice dynamics of 4H-SiC by inelastic x-ray scattering, J. Serrano *et al*, Mat. Sci. Forum 433-4, 257 (2003).



Phonon dispersion relations of 4H-SiC measured (circles) along the A-H-L direction. The solid lines correspond to the calculated dispersions. r.l.u. stands for *relative lattice units*.