



	Experiment title: Determination of the lattice dynamics of wurtzite InN by grazing incident inelastic x-ray scattering	Experiment number: HS-3201
Beamline: ID28	Date of experiment: from: May 9 th , 2007 to: May 15 th , 2007	Date of report: 31/08/2021
Shifts: 24	Local contact(s): Jorge Serrano	<i>Received at ESRF:</i>
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Report:

We performed room temperature, grazing incidence, inelastic x-ray scattering (IXS) experiments on a 5 micron thick $5 \times 7 \text{ mm}^2$ surface wurtzite InN thin film in order to investigate both the phonon dispersion relations and the elastic tensor.

The sample was obtained by MBE growth at $600 \text{ }^\circ\text{C}$ on a (0001) sapphire substrate using a GaN buffer layer.

The grazing incident IXS experiments were conducted at beamline ID28 at ESRF. We employed backscattered monochromatic 17.794 keV x-rays deflected by a flat platinum coated mirror to achieve grazing incidence on the sample, yielding 3 meV energy resolution and using a toroidal mirror to provide a spot size of $60 \times 250 \text{ }\mu\text{m}^2$ (vertical x horizontal). A 5-analyzer configuration was employed to maximize sampling on the Brillouin zone in each acquisition. The experiments were conducted with the guide of our own ab-initio calculated phonon dispersion relations and scattering intensities. This turned out to be essential to ascertain the scattering configurations with highest signal and optimized the beamtime use.

These experiments provided the first reported data on the phonon dispersion relations of wurtzite InN, particularly for acoustic modes and low energy optical modes. Figure 1 displays the phonon dispersion relations for the main high symmetry directions, highlighting the excellent overall agreement between the ab-initio calculated dispersion (solid and dashed lines) and the IXS data (symbols).

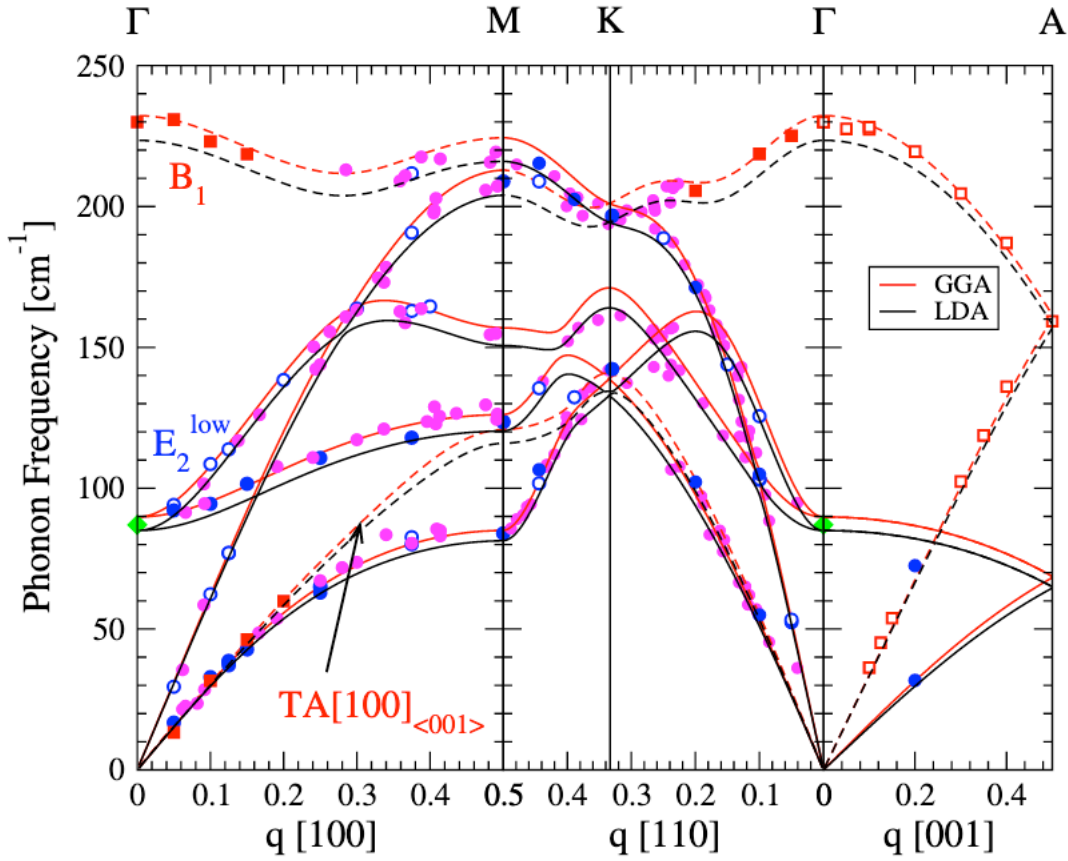


Figure 1: Acoustic and low-energy optic phonon dispersion relations of wurtzite InN along the main symmetry directions. Open and solid symbols display IXS data corresponding to longitudinal and transverse modes, respectively, except for the solid circles that display IXS data obtained using mixed transverse and longitudinal polarizations. The black (red) curves plot results obtained from LDA (GGA) *ab initio* calculations. Modes polarized along the $h001i$ direction of the BZ are represented by (red) squares and dashed lines, whereas in-plane polarized modes are represented by (blue) circles and solid lines. Reported in Ref. [1].

Elastic constant	IXS GPa	Other experiments GPa, from Ref. [2]
C_{11}	225(7)	190(7)
C_{12}	109(8)	104(3)
C_{13}	108(8)	121(7)
C_{33}	265(3)	182(6)
C_{44}	55(3)	10(1)
C_{66}	58(2)	43(5)

Information on the elastic constants was also extracted for all different symmetry directions thus yielding the **complete elastic tensor for wurtzite InN** (see Table 1)

Table 1: Elastic stiffness constants of wurtzite InN obtained from the IXS data for the acoustic branches, compared to data obtained from temperature dependence of XRD broadening [2].

The results of these experiments were reported in a regular publication on Physical Review Letters [1], and represent as well the first phonon dispersion data reported on epitaxially grown thin films, to the best of our knowledge.

References:

[1] *InN Thin Film Lattice Dynamics by Grazing Incidence Inelastic X-ray Scattering*, J. Serrano *et al.*, Phys. Rev. Lett. **106**, 205501 (2011).

[2] *Determination Des Constantes Elastiques Des Cristaux Hexagonaux A Partir Des Mesures Des Deplacements Dynamiques Des Atomes*, U. Sheleg And V. A. Savastenko, Izv. Akad. Nauk SSSR, Neorg. Mater. **15**, 1598 (1979) [Inorg. Mater. (USSR) **15**,1257 (1979)].