ESRF	**Experiment title:** Lattice Dynamics of Hexagonal Boron Nitride (h-BN) by Inelastic X-ray Scattering	**Experiment number**: HS-2915
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Report:

We report here measurements of the phonon dispersion relations of hexagonal BN (h-BN) by inelastic x-ray scattering (IXS) at room temperature. These measurements were performed at the beamline ID28 using monochromatic light of 17.794~keV (15.816~keV) and an energy resolution of 3~meV (5~meV) for the acoustic (optic) phonons. With this aim, we employed several h-BN single crystals that consist on platelets of 500X200 microns surface and approx. 50 micron thickness. The aid of first principles calculations was useful to ascertain the best scattering geometries for the experiment. The phonon dispersion relations were obtained along the main symmetry directions, i.e., **Γ -**M (100), **Γ -**K-M (110), and **Γ**-A (001). Acoustic branches along particular directions, such as **<**112**>** and **<**1 1 36**>**, were also investigated in order to determine the full set of elastic constants.

Hexagonal BN has a unit cell with 4 atoms and therefore shows 12 branches in the phonon dispersion relations. There are five independent elastic constants for the hexagonal system, which can be obtained from the slopes of the acoustic branches at small momentum transfer along specific directions. Before this experiment, the complete set of elastic stiffness constants had not been reported in the literature, probably due to the difficulties to grow a large single crystal suitable for Brillouin spectroscopic measurements.

We have obtained an excellent agreement between the elastic constants and those reported by calculations and with the rather limited experimental data reported in the literature; the details about the determination of the elastic constants on h-BN by IXS have been published in Ref. [1]. Figure 1 summarizes the results obtained for the phonon dispersion relations of h-BN. Contrary to HREELS data taken on a monolayer of h-BN deposited on Ni(111) [2], we observe a splitting of 35 meV between the transverse acoustic and optic modes at the K-point. Besides this, significant differences were found also for the high energy branches. Except for the longitudinal optic branches and the rather flat high energy phonon dispersion along the c-axis, we obtained a complete picture of the lattice dynamics of h-BN. The agreement with the theoretical calculations is outstanding, as well as with previous theoretical data reported in the literature [3].

In conclusion, we have determined the complete set of elastic stiffness constants of hexagonal BN by IXS measurements. Besides this, the phonon dispersion relations have been obtained, showing significant differences with the only experimental data available, obtained by HREELS. The measurements were performed with the aid of *ab initio* calculations whose results display an excellent agreement with our data. A manuscript summarizing our findings is under preparation.

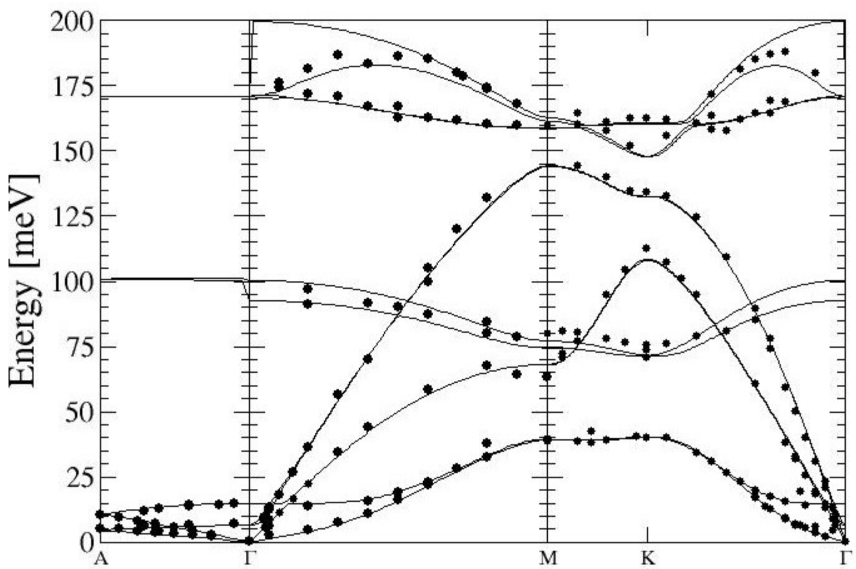

Fig. 1: Phonon dispersion relations of hexagonal BN. Full circles display IXS data, whereas the solid curves are the result of first principles calculations.

[1] A. Bosak et al., *Elasticity of hexagonal boron nitride: inelastic x-ray scattering measurements*, Phys. Rev. B **73**, 041402 (2006).

[2] E. Rokuta et al., *Phonon dispersion of an epitaxial monolayer film of hexagonal boron nitride on Ni(111)*, Phys. Rev. Lett. **79**, 4609 (1997).

[3] G. Kern et al., *Ab initio calculations of the lattice dynamics and the phase diagram of boron nitride*, Phys. Rev. B **59**, 8551 (1999).