ESRF	**Experiment title:** Momentum transfer dependent valence excitations in hexagonal boron nitride	**Experiment number:** HE2446
Beamline: ID16	**Date of experiment:** from: 20.6.2007 to: 25.6.2007	**Date of report:** 5.2.2008
Shifts: 15	**Local contact(s):** Dr. S. Huotari	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
S. Galambosi*, K. Hämäläinen*, J.A. Soininen
Division of Materials Physics, Department of Physics, POB 64, 00014 University of Helsinki, Finland

Report:
We have studied the valence electron excitations of hexagonal boron nitride (hBN) using inelastic x-ray scattering (IXS). The experiment is part of an extended study combining x-ray diffraction, IXS and GW-BSE calculations aimed at clearing up the current ambiguity related to the valence electron structure of hBN.

Despite of various theoretical and experimental studies, the valence electron structure of hBN is not well understood. A widely dispersed band gap energy ranging from 3.6 eV to 7.1 eV can be found in the literature and both direct and indirect band gaps have been reported. Previous experiments were partly hindered by the lack of large enough and defect-free crystals. Moreover, hBN can be formed by various stacking sequences of the hexagonal BN-layers [1], which has to be taken into account in the theoretical calculations.

The valence excitation spectra of hBN were studied using the eV-resolution spectrometer situated at ID16. We used a large single crystal sample available only recently due to the advances in the crystal growing techniques [2]. The valence excitation spectrum spanning an energy range of 80 eV was recorded along several directions of the crystal structure employing various values of momentum transfer. Figure 1 shows the evolution of the IXS spectra using a set of momentum transfer values ranging from 0.25 a.u. to 3.35 a.u. along the ΓK direction. The first 14 eV of the excitation spectra were recorded at a finer energy step in order to address the band gap controversy of hBN.

As the momentum transfer vector had to be positioned exactly on discrete points in the reciprocal lattice of hBN, we could utilize the data only of a single analyzer crystal of the multianalyzer array setup. Nevertheless, the high incident intensity available on ID16 enabled us to collect IXS spectra using a fine grid of momentum transfers. All spectra were collected using a Si 110 crystal utilizing the (440) reflection in a backscattering geometry resulting in an energy resolution of 0.60 eV at the incident energy of 6.46 keV.

The analysis of the IXS spectra together with the subsequent x-ray diffraction data is under way. Based on the preliminary data analysis, the quality of the experimental IXS data certainly merits the publications of the results.

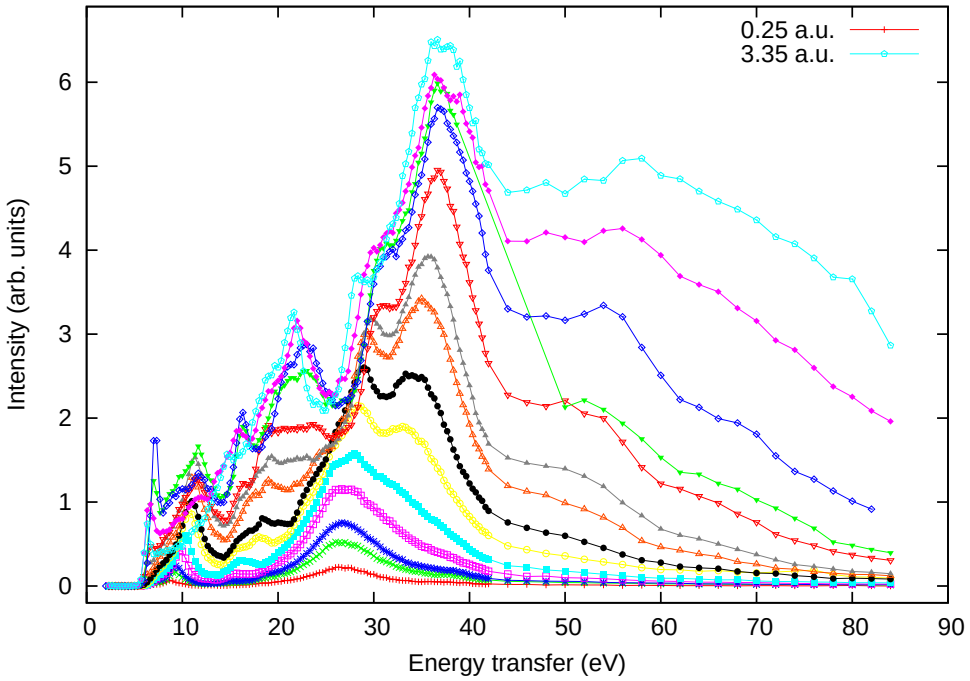

Figure 1: The momentum transfer dependence of the valence excitation spectrum of hBN along the ΓK direction.

[1] N. Ooi, A. Rairkar, L. Lindsley and J. B. Adams, J. Phys.: Condens. Matter **18**, 97 (2006).

[2] T. Taniguchi and S. Yamaoka, J. Cryst. Growth **222**, 549 (2001).