

# Non-Resonant Inelastic X-Ray Scattering Study of Cubic Boron Nitride

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Beamline(s): X21

**Introduction:** During the recent years boron nitride has been extensively studied via numerous experimental techniques because it exhibits several fascinating characteristics such as semi conducting properties, extreme hardness, high thermal conductivity and large band gap. The optical properties of cBN have also drawn both experimental [1] and theoretical interest [2].

**Methods and Materials:** The double differential cross section of inelastic x-ray scattering is directly proportional to the dynamic structure factor  $S(q,\omega)$ , where  $q$  and  $\omega$  are the momentum and energy transfer, respectively. The dynamic structure factor can be written in terms of the macroscopic dielectric function, which describes the response of the system to the total macroscopic electric field. The fact, that non-resonant inelastic x-ray scattering (NRIXS) directly probes the dynamic structure factor, makes it possible to experimentally obtain the momentum and energy transfer dependence of the macroscopic dielectric function.

We have conducted a combined experimental and theoretical study of dynamic structure factor of single crystal cubic boron nitride (cBN) using non-resonant inelastic x-ray scattering. The experimental part was carried out on beamline X21A3 performing the energy scans at several momentum transfers on the three main crystallographic axes (100, 110 and 111). The data was normalized to absolute scale using the  $f$ -sum rule [3].

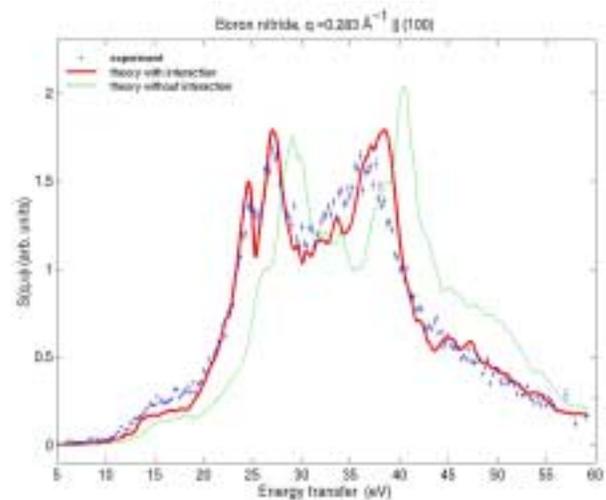
**Results and Conclusions:** The experimental data are compared with results of a recently developed *ab initio* calculation scheme [4], which takes into account the interaction between the excited electron and the hole. The agreement between the experiment and theory is excellent, as long as the electron-hole interaction is taken into account. The importance of this interaction is emphasized in the figure, which shows comparison of theory with and without the electron-hole interaction correction between the experimental data set.

We also show, that using low momentum transfer, the experimental dynamic structure factor can be directly related to optical absorption and reflectivity measurements.

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**Figure 1.** Experimental dynamic structure factor of cubic boron nitride along 100 direction (symbols) compared with the theoretical calculation with (thick solid/red line) and without (thin solid/green line) electron-hole interaction.