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Names and affiliations of applicants (* indicates experimentalists):

A. Mattila*, S. Galambosi*, J. A. Soininen, S. Manninen and K. Hämäläinen*

Division of X-ray Physics, Department of Physical Sciences, University of Helsinki, Finland

S. Huotari* and G. Vanko*

ESRF, Grenoble, France

Report:

The discovery of relatively high critical temperature $T_C \approx 39$ K of superconductivity in MgB_2 has sparked off considerable interest on the properties of this and other binary metal compounds. From these studies a picture of MgB_2 as a conventional BCS type superconductor has emerged. The large hole density of states near the Fermi level provided by the boron σ(p)–bands has been identified to be the key contributing factor to high T_C. This picture is consistent with the destruction of the superconductivity with the filling of B σ-band holes by Al substitution. However, the details of the empty σ-bands are still under debate.

In this experiment we probed the empty electronic states of boron in single crystal MgB_2 using Non-Resonant Inelastic X-ray Scattering (NRIXS) utilizing the ID16 eV-resolution spectrometer. NRIXS at low momentum transfer is equivalent to conventional X-ray Absorption Spectroscopy (XAS), thus providing direct information on the empty electronic states. As in XAS with single crystal samples in NRIXS the orientation of the probed empty states can be selected by controlling the orientation of the momentum transfer $\vec{q}$ relative to the crystallographic orientation of the sample. Unlike XAS however, NRIXS allows also to probe the spatial symmtery of the empty states by tuning the absolute value of the momentum transfer. At high momentum transfer values monopole and higher order transitions start to dominate over dipole transitions, thus increasing the contribution from *s* and *d* symmetry empty states.

We measured the NRIXS spectra at three different scattering angles corresponding to momentun transfer values of 2.1 Å^{-1}, 4.0 Å^{-1} and 9.7 Å^{-1} as a function of energy transfer at the boron K-edge. The measurements were done with two orientations of the crystal, with the momentum transfer $\vec{q}$ parallel to [100] or [001] directions. The energy transfer scans were performed using the so-called inverse energy scan technique, where the scattered photons are analyzed at a fixed energy and the energy transfer is tuned by changing the energy of the incident photons. The energy resolution was 1.0 eV for the two lower momentum transfer spectra and 1.4 eV for the 9.7 Å^{-1} spectra.

Figures 1. and 2. show the $\vec{q}$-dependence of the NRIXS signal with the momentum transfer aligned along the different crystal directions. The inelastic contributions from the valence electrons have been subtracted from the spectra. The spectra reveal a considerable anisotropy of the empty bands near the Fermi level. A dependence on the absolute value of $\vec{q}$ is clearly observed in the spectra, being quite pronounced in the spectra recorded with the $\vec{q}$ aligned along the [001] direction (*c*-axis). This dependence reflects the increasing contribution from *s* symmetry finals states at higher momentum transfer.

We have modelled the spectra using *ab initio* multiple scattering formalism. The calculations reveal a considerable core-hole effect, precluding the use of ground state band structure calculations for the analysis of the spectra. The directional dependence of the spectra is well reproduced in the calculation and further effort is on the way to also study the $\vec{q}$-dependence using computational approaches. A manuscript on the results is under preparation.

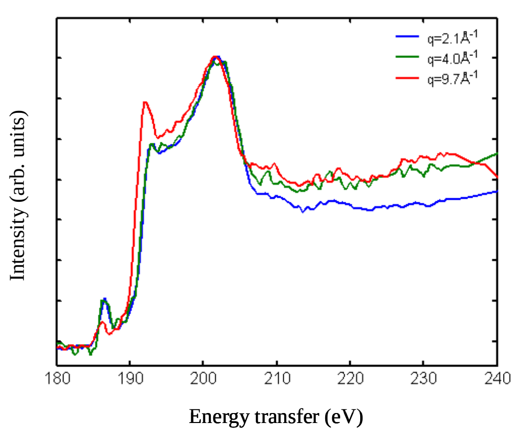

Fig. 4. NRIXS spectra with *q* aligned along the *ab*-plane.

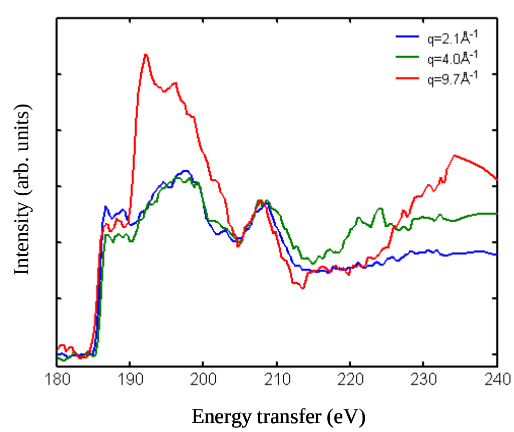

Fig. 5. NRIXS spectra with *q* aligned along the *c*-axis.