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An Accurate MgB_2 Boron K x-ray Absorption Edge

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Beamline: U7A

Introduction: Soft x-ray absorption spectroscopy (XAS), using fluorescence yield, was used to study the boron K near edge in polycrystalline MgB_2 (which has a high superconducting transition temperature, Tc=40 K). An accurate band structure should be readily calculated for the relatively simple MgB_2 structure. The theory is, in principle, verified by a straightforward comparison with boron K edge structure. A complication is that impurity, or second phase, components can occur in MgB_2. Impurities such as boron oxides or nitrides consist solely of light elements, and may be amorphous or poorly crystallized. Evidence for impurities in diffraction or chemical analysis is not strong. However, previous soft x-ray studies of the boron K edge in MgB_2 have shown evidence for notable impurity features. In this work we obtain the boron k-edge of a clean MgB_2 polycrystalline sample.

Methods and Materials: A composite sample, consisting of MgB_2 crystallites within a protective Mg matrix, was prepared using an excess of Mg. The MgB_2, effectively coated by Mg, is protected from reaction with air. After the sample was introduced into the experimental vacuum chamber, the sample face was abraded to obtain a clean surface for study. The experiment utilized incident photons with an energy resolution of 0.1 eV. Fluorescence yield data were obtained using a gas-proportional counter. Partial electron yield data were obtained in some cases. The MgB_2 partial density of states (PDOS) and XAS spectrum were calculated using the FLAPW method within the WIEN97 code. Calculated PDOS and XAS spectra are comparable to other studies.

Results: Figure 1 shows two boron K XAS spectra for the composite MgB_2. The lower curve represents MgB_2 powder. A prominent feature at ~193.6 eV is probably due to boron oxide impurites on the surface, and an additional feature near 191.5 eV may represent boron nitride. After scraping (upper curve) the feature 191.5 eV is essentially removed while that at 193.6 eV is much reduced in size. Additional measurements show the feature at 193.6 eV to increase slowly in size with time as impurities in the high vacuum chamber react with the MgB_2 surface. Comparison with the calculated XAS spectrum (Figure 2) shows good agreement below about 194 eV, but only qualitative agreement at higher energies.

Conclusions: XAS measurements play two important roles in the study of MgB_2. The x-ray absorption probe is a sensitive probe for the presence of impurity phases that are not otherwise well documented. The second role is for comparison with the fundamental electronic band structure calculations for this material

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References: Y. Zhu et al., "Unraveling the Symmetry of the Hole State near the Fermi Level in the MgB_2 Superconductor," Phys. Rev. Lett. **88** (2002) 247002-1 - 247002-4, and references therein.

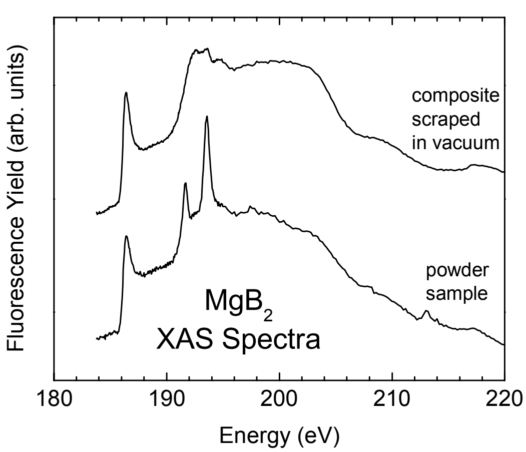

Fig. 1. Boron K edges for powder sample (lower) and scraped composite (upper) MgB_2.

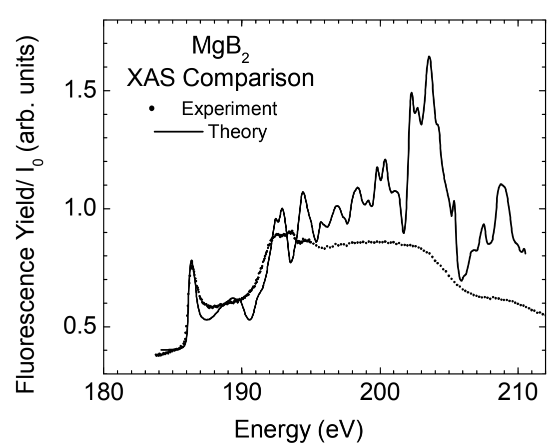

Fig. 2. Comparison of composite MgB_2 XAS spectrum with calculated edge structure.