Resonant magnetic x-ray scattering study of K₂ReBr₆

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Introduction

 K_2 ReBr₆ crystallizes in the antifluorite structure with space group Fm3m with a structure composed of a face-center cubic arrangement of ReBr₆ octahedra with interstitial K⁺ ions [1]. The material undergoes a magnetic phase transition to a long-range ordered antiferromagnetic state where neighboring planes of spins are aligned antiparallel with parallel alignment within a plane (so called Type I antiferromagnet) [2]. The extended nature of the electron distribution associated with the magnetic 5d electrons often leads to large covalency effects in these materials, and these effects have been a topic of interest for a number of years [3]. These effects are often rather striking as seen in the compound K₂IrCl₆, where neutron diffraction measurements of the magnetic form factor indicated that about 30% of the Ir⁴⁺ moment was actually delocalized and located on the surrounding Cl⁻ ions [4].

A project was initiated to study these covalency effects in K_2ReBr_6 using resonant magnetic x-ray scattering. Resonant enhancements associated with the L edges of 5d ions have not been studied extensively and, hence, these measurements may also help to extend the applicability of this technique to a new family of compounds. In addition, we hope to be able to observe a resonant enhancement associated with the Br K-edge, which, by comparison to the Re L-edge scattering, should provide a novel method for examining covalency effects in these compounds.

Results and Discussion

A preliminary measurement was performed on a singlecrystal sample of K₂ReBr₆ in the UNI-CAT 33-ID beamline. The sample was attached to the cold finger of a closed-cycle He refrigerator that was then inserted into a Huber four-circle diffractometer. The low-temperature measurements were complicated by the presence of a number of structural domains resulting from a higher temperature structural phase transition. The low-temperature structure was later found to be monoclinic with space group P12₁/n1 [5] in contrast to the room-temperature cubic structure with space group Fm3m. Despite this complication, we were able to clearly observe resonant magnetic x-ray scattering associated with the L_{III} edge of Re. This scattering is shown in Fig. 1 where the intensity of the magnetic (7 7 0) reflection can be seen to peak sharply at the absorption edge energy (Fig. 1a) and is also seen to disappear upon warming through the Néel temperature (Fig. 1b). In addition, resonant magnetic scattering was also observed at the Re L_{II} absorption edge. These observations represent one of the first measurements of resonant magnetic scattering associated with the L-edges of 5d electron atoms and we hope that these observations will act to extend the use of the technique to a new family of materials. Unfortunately, due to geometrical constraints, we

were unable to extensively search for Br K-edge scattering and we hope to expand these measurements in the future.



Figure 1: (a) Energy dependence of the (770) magnetic reflection showing resonant enhancement at the Re LIII edge. (b) The temperature dependence of the (770) magnetic reflection which disappears on warming through the Néel temperature.

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