

LOCAL MAGNETISM AND STRUCTURAL DISTORTIONS IN BaIrO_3 INDUCED BY SR-DOPING AND HIGH PRESSURES

Maria A. Laguna-Marco¹, Daniel Haskel¹, Narcizo Souza-Neto¹, Yuan-Chieh Tseng¹, Gang Cao², and Shalinee Chikara²

¹Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439; ²Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506

INTRODUCTION

Because of their wide variety of electronic ground states, namely superconductivity, ferromagnetism, multiferroicity, metallic/insulating together with their numerous applications, perovskites and their derivatives are amongst the most studied compounds in material science. Recent studies have shown that layered iridates such as BaIrO_3 share a number of unique features including high temperature weak ferromagnetism (Curie temperature $T_C = 175$ K), charge-density-wave formation and a temperature-driven transition from a metallic to an insulating ground state (1,2). It has also been found that doping small amounts of Sr into BaIrO_3 induces strong changes in the magnetic and transport properties. Unlike the more localized nature of 3d electronic orbitals in transition metal ions, the greatly extended Ir-5d orbitals generate strong electron-lattice coupling and the magnetism and electronic structure are thus critically linked to the lattice degrees of freedom. However, the mechanism responsible for the drastic decrease of T_C with Sr doping is still unclear. There is no consensus yet as to whether the main effect of doping is to contract the lattice volume (Sr²⁺ ions are smaller than Ba²⁺ ions) or to induce IrO₆ octahedral Jahn-Teller like distortions and/or octahedral tilts affecting Ir-O-Ir angles. Each of these possibilities leads to a different interpretation for the effect of Sr doping on magnetism. This work explores how chemical pressure (Sr-doping) affects the magnetism and local structure of BaIrO_3 by comparing with the effect of applying high hydrostatic pressure to contract the lattice. XAFS and XMCD techniques are used to study whether a uniform volume contraction can account for the destruction of weak ferromagnetism and the insulator-metal transition observed with Sr doping or whether local structural distortions ought to be considered in explaining these phenomena. A further point under study is the role that orbital ordering may play in the magnetic behavior of these compounds. XMCD can also contribute to clarify this point as it probes separately the orbital and spin 5d magnetic moments, while this information is hidden to macroscopic measurements.

EXPERIMENTAL

Sr-doped samples were grown as single crystals using flux techniques (1). BaIrO_3 was grown as a polycrystalline sample. X-ray diffraction (XRD) confirmed the single-phase nature of the samples. In addition, the lattice parameters change linearly with Sr doping indicating that Sr incorporates into the lattice. The x-ray measurements were carried out at beamline 4-ID-D of the Advanced Photon Source at Argonne National Laboratory. Circularly polarized x rays were generated by phase-retarding optics (3) and the XMCD

measured by modulating the x-ray helicity. Spectra were recorded in transmission mode under an applied magnetic field of 0.4T. For the measurement at ambient pressure homogeneous layers of the powdered samples were made by spreading fine powders of the material onto an adhesive tape. The thickness and homogeneity of the samples were optimized to obtain a total absorption jump of ~ 1 at about 50 eV above the edge. For the high pressure experiments the powders were mixed with ruby (calibrant) and dispersed in silicon oil which was used as hydrostatic pressure medium. A copper-beryllium diamond anvil cell DAC was used to apply pressure. The DAC was mounted on the cold finger of a He-flow cryostat, itself placed between the pole pieces of an electromagnet. The pressure could be varied *in situ* during low-temperature measurements without having to remove the cell from the cryostat. Detailed information about the experimental setup can be found in (4).

RESULTS

XMCD spectra recorded at the Ir $L_{2,3}$ edges show a reduction of both magnetic ordering temperature T_C and saturation magnetization with Sr doping in agreement with macroscopic magnetization measurements. However, we have found that, contrary to other Ir systems (5), the XMCD signals at both edges present the same sign indicating that a large orbital moment is present in the Ir 5d band. This is confirmed by applying sum-rules analysis (6) which yields an orbital-to-spin $\langle L_z \rangle / \langle S_z \rangle$ ratio larger than 1 for the Ir 5d band. On the other hand, XMCD carried out under pressure indicates that a relatively low applied pressure of 1.2 GPa is enough to suppress the magnetic ordering in BaIrO_3 . Our results seem to indicate that a uniform volume contraction cannot fully account for the destruction of the weak ferromagnetism present in BaIrO_3 . Further XMCD and XAFS work under pressure is in progress to clarify this point and to elucidate the role of the large orbital moment in the weak ferromagnetic ordering displayed by this compound.

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