Orbital Polarization and X-ray Absorption Linear Dichroism in Transition-Metal Oxides

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We discuss the recent theories and experiments on the orbital polarization and x-ray absorption linear dichroism (XLD) in perovskite-type 3d transition-metal oxides. In 2000, we predicted an expected XLD in Mn L_{23} absorption for $LaMnO_3$ by the exact diagonalization of a single-ion model including the 3d-3d and 3d-2p multipole coulomb interactions and crystal field [1]. In $LaMnO_3$, three of Mn 3d electrons occupy the triply degenerate t_{2g} state and one electron occupies the doubly degenerate eg state and the C-type antiferro-orbital ordering (AF-OO), i.e., alternate arrangement of orbital polarization is reported. We showed that the reported AF-OO contributes to the XLD signal unlike the case of antiferromagnets with vanishing XMCD due to cancellation between two sublattices. We also showed that the basic XLD pattern is only one irrespective of AF-OO and ferro-OO in the doubly degenerate case. These results are fully utilized in the analysis of observed Mn $L_{2,3}$ XLD of LaSrMnO4 with ferro-OO and half-doped $La_{0.5}Sr_{1.5}MnO_4$ [2]. Especially, in $La_{0.5}Sr_{1.5}MnO_4$, where $3x^2$-$r^2/3y^2$-r^2 AF-OO of Mn^{3+} is so far proposed, the predominantly z^2-x^2/y^2-z^2 AF-OO is concluded for the observed XLD.

The study on the relation between XLD and the orbital polarization was extended to ferromagnetic $YTiO_3$, which is rare in Mott insulators and AF-OO among the triply degenerate Ti 3d states is reported. The Jahn-Teller distortion (JTD) of TiO_6 octahedra accompanied by the AF-OO and the so-called $GdFeO_3$-type tilting is observed in this system. Due to symmetry, the four kinds of polarizations c_1zx+c_2xy, c_1zx-c_2xy, c_1yz+c_2xy and c_1yz-c_2xy are reported to be alternately arranged and there have been however scatterings of c_1 (or c_2) value among observed data other than XLD. The measurement of Ti L_{23} XLD and our analysis [3] determine c_1 (c_2) of ~0.8 (~0.6), which is crucial to the origin of ferromagnetism of this system.

[1] H. b. Huang, t. Shishidou and T. Jo, J. Phys. Soc. Jpn. **69** (2000) 2399.

[2] D. J. Huang et al., Phys. Rev. Lett. **92** (2004) 087202.

[3] F. Iga et al., Phys. Rev. Lett. **93** (2004) 257207.