X-ray absorption spectroscopy study of YMnO$_3$

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Hexagonal perovskite YMnO$_3$ is a well-known material where both magnetism (AFM, $T_N \approx 80 \text{K}$) and ferroelectricity ($T_C \approx 900 \text{K}$) co-exist. These two properties were traditionally believed to have different origin, since the ferroelectricity usually occurs in nominal $d^0$ transition metal system whereas the magnetism does in compounds of occupied $d$− or $f$− electrons. To explain this coexistence in YMnO$_3$, Filippetti et al. [1] proposed a model which argues the empty $d_{3z^2-r^2}$ level along $c$-axis alone strongly hybridizes with $p$-orbital of apical oxygen. We present polarization-dependent XAS results to support their prediction with more implications.

The room-temperature X-ray fluorescence yield was measured at EPU6 beamline in Pohang Accelerator Laboratory. Single-crystalline YMnO$_3$ platelet was prepared carefully to be of axes [0001] $\times$ [110], so that the incident beam polarizations were along those directions.

Each of the oxygen K-edge spectra shows distinct charge-transferred features: along $c$-axis, $pd\sigma : d_{z^2} \downarrow - O_Tp_z$ and $pd\pi : d_{xz} \downarrow - O_{pp}p_z$ with interval $\sim 1.6\text{eV}$; along ab-axis, $pd\sigma : d_{xy} \downarrow - O_{pp}p_x$ and small feature of $pd\sigma : d_{z^2} \downarrow - O_Tp_z$ with interval $\sim 1.3\text{eV}$.

These results could be compared with LDA+U calculation [2], and with Second Harmonic Generation(SHG) data. (e.g. [3])