The surface study of ReFeO$_3$ (Re=Lu, Yb) thin films by X-ray Photoemission Spectroscopy and Density Function Calculation

SHI CAO, TULA PAUDEL, KISHAN SINHA, XUANYUAN JIANG, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA, WENBIN WANG, Department of Physics, Fudan University, Shanghai, 200433, China, EVGENY TSYMBA, XIAOSHAN XU, PE-TER DOWBEN, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA — The rare-earth ferrites, ReFeO$_3$, may have a large magneto-electric response, with high surface/interface polarization, thus the surfaces are of considerable interest. We have characterized the surfaces of hexagonal ReFeO$_3$ (Re= Lu, Yb) and orthorhombic LuFeO$_3$ thin films by angle resolved X-ray photoemission spectroscopy (ARXPS) and compared with density function theory (DFT). The surfaces will terminate in either Fe-O or Re-O depending on whether in the hexagonal or orthorhombic phase of the rare earth ferrite, but consistent with the expectations of DFT. The orthorhombic or hexagonal phases of these rare earth ferrites have the Fe in different crystal fields, which in turn affects the of Fe-O ligands. These changes in electronegativity are experimentally evident as differences in the Fe 2p core level photoemission satellite features. Surface preparation also effects surface termination and will be discussed.

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