Unoccupied band splitting in metallic epitaxial IrO$_2$ film due to SOC

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Materials based on 5d transition metal oxides with strong spin-orbit coupling (SOC) have been predicted to exhibit a variety of nontrivial electronic properties, such as the Mott insulator, Weyl semimetallic state, topologically insulating behavior, and novel superconducting states [1]. Moreover, heavy transition metals and their oxides, such as IrO$_2$ have been receiving increasing attention in the as promising materials for application in spintronics [2] thanks to pronounced SOC effects in these compounds.

In connection with this, a deep understanding of the ground state of such materials is of high value. Particularly, an ongoing controversy about the role of the strong SOC in the metallic state of IrO$_2$ needs to be resolved. A conventional interpretation of a metallic state of this material does not involve SOC [3], however the result of GGA+U+SO calculations demonstrated a dominant role of strong spin-orbit coupling in IrO$_2$ [4]. A key piece of information would be provided by the results of the experimental studies of the band structure of this compound.

We have studied the electronic structure of IrO$_2$ using optical spectroscopy and X-ray photo electron spectroscopy. XPS and UPS measurement were done on single phase, epitaxial IrO$_2$ film, reproducing the general features of a recent band structure calculation. The optical measurement for E//c axis and E ⊥ c axis at room temperature have been performed in a photon energy range between 3.5 meV ~ 5.5 eV. A clear peak near 0.5 eV has been observed on our optical conductivity spectra. These results can explain a formation of a band above the Fermi level due to SOC and are in good agreement with recent GGA+U+SO band structure calculations.