Structure-property Relationships in Pure and Doped Epitaxial Tungsten Trioxide Thin Films

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Abstract

The primary objective of this project is to investigate the structure-property relationships of well-defined epitaxial tungsten trioxide (WO3) films with and without dopants, and thereby provide fundamental insights into the catalytic and photocatalytic properties. Our hypothesis is that through systematic studies of molybdenum (Mo) and nitrogen (N) doped WO3 films, we can understand the fundamental principles and determine the extent to which: (1) Mo doping can change the alcohol dehydration chemistry of WO3, and (2) N doping can redshift the 2.8 eV band gap deeper into the visible region. It is anticipated that such a fundamental understanding of the structure-property relationship in epitaxial pure and doped films will help us to derive a general model that will be applicable to a large class of dopants in WO3. We propose to grow structurally excellent epitaxial WO3 films on appropriately symmetry- and lattice-matched oxide substrates using the next-generation ozone-assisted molecular beam epitaxy (MBE) system equipped with high-sensitivity *in-situ* atomic absorption flux sensors recently developed at PNNL.

The team consisting of PNNL staff and university collaborators will take full advantage of the unique suite of capabilities available at EMSL and collaborators' sites, including deposition and microfabrication, spectroscopy and diffraction, microscopy, and high performance computing. The proposed research is of significant interest in catalysis and photocatalysis, and fits very well with the EMSL mission, in particular, the integration of experiments and theory to solve complex scientific problems.