# Epitaxial Growth and Properties of Nanoscale Oxides for Spintronics

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**Project Summary:**

The discovery and utilization of new semiconducting materials that are ferromagnetic at room temperature is required for the realization of spintronics – a potentially very important development in electronics and magnetics technology. In spintronics, the spins of electrons, holes, ions, and/or atoms are utilized to develop faster, smaller, and less power dissipative ways of processing, transmitting, and storing information. Applications range from on-chip integration of magnetic storage and electronic processing functions over nanometer length scales to quantum computing. In all cases, the essential physics occurs over length scales that are of the order of a few to a few tens of lattice spacings in crystalline solids. Over the next year, we propose to continue our work in the synthesis and properties of candidate oxide semiconductors that may be ferromagnetic at ambient temperature. These include $Mn_xZn_{1-x}O$ ($x < \sim 0.35$) and $Co_xTi_{1-x}O_2$ anatase ($x < \sim 0.8$).

The anatase phase of $TiO_2$ is grown at PNNL using oxygen plasma assisted molecular beam epitaxy (OPA-MBE). TiO2 is grown on three different substrates; lanthanum aluminate, $LaAlO_3$ (001) (lattice mismatch –0.26%), strontium titanate $SrTiO_3$ (001) (lattice mismatch –3.1%). For comparison, rutile films were grown under the same conditions on rutile (110). The films are studied *ex situ* and thus must be cleaned. Surface contaminants were removed by annealing the sample at 530°C, first in ~$5x10^{-5}$ torr $O_2$, then in vacuum; which removes 90% of the contaminating carbon. No sputtering is required.

A key element in predicting the magnetic and catalytic properties of anatase is knowledge of the electronic band structure. We do this by analyzing the samples with various techniques such as x-ray photoelectron spectroscopy (XPS), photoelectron spectroscopy (PES), and near-edge x-ray absorption fine structure (NEXAFS). The XPS and PES can be performed at UW, while the XPS, PES, and NEXAFS are all done at LBNL's Advanced Light source (ALS) in Berkeley, CA. XPS is an element specific technique for composition, PES is useful for valence band mapping, and NEXAFS can distinguish different crystal structure and the local atomic environment.

While we have gathered much information from the above techniques, there are still more questions to be answered. In the future, we plan to study these films using Photothermal Deflections Spectroscopy (PDS) to determine any states in the optical gap. We will also study the growth and nucleation of anatase and Co doped anatase on LAO and STO substrates with scanning probe microscopy. Both experimental techniques will be carried out at UW.

**Publications, Presentations and Proposals:**

"Electronic Structure of Thin Film Anatase TiO2: A Candidate Spintronics Material." D. A. Schmidt, J. A. Adams, A. A. Bostwick, S. A. Chambers, M. A. Olmstead. 2002 Nanotech Workshop, UW, Seattle, WA; 2002 PNW-AVS, Vancouver, WA; 2003 CDO Networking Day, UW, Seattle, WA

**Selected Figures:**

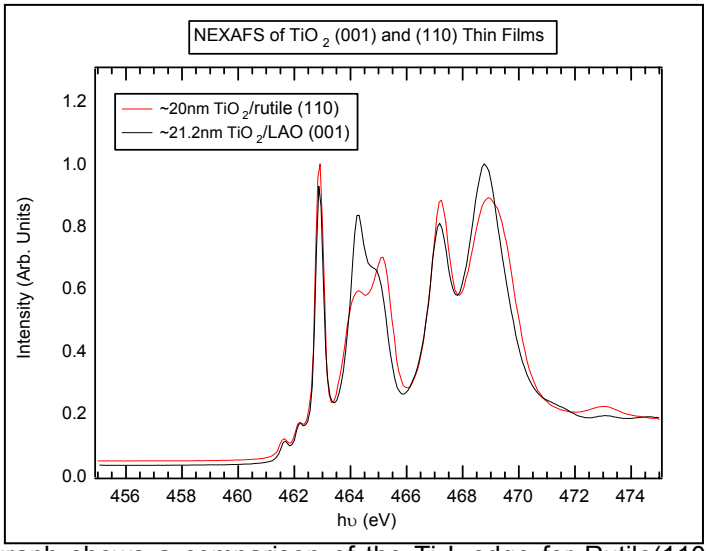


**Figure 1:** This graph shows a comparison of the Ti L-edge for Rutile(110) and Anatase(001) films. The two curves are similar with some minor differences. The pre-edge structure is the same in both films, and only the relative intensities of other peaks vary. This indicates that the distorted octahedral environment in anatase does not drastically change the crystal field interactions. Note the change in shoulder position of the fourth peak: on the right with anatase, and on the left for rutile, distinguishing the two crystal structures.

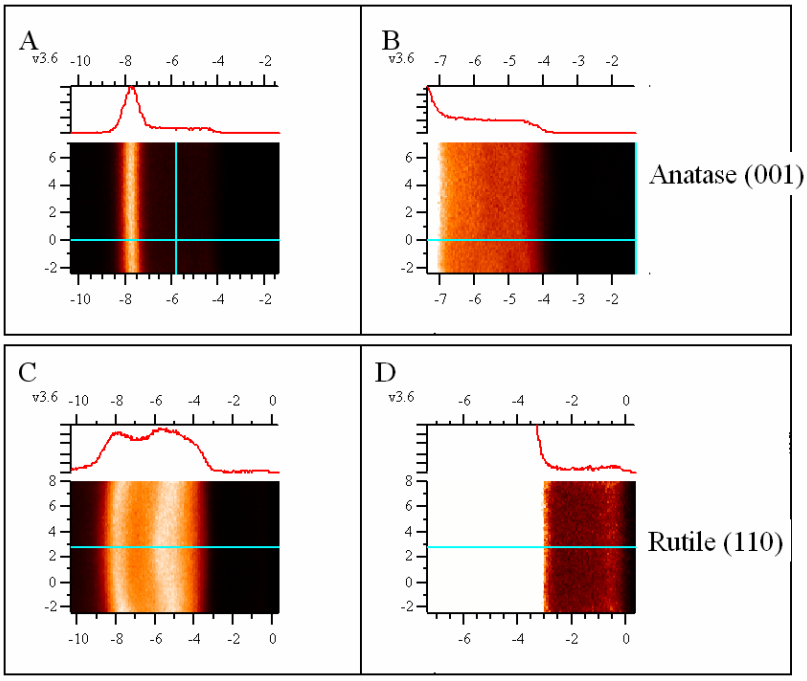


**Figure 2:** Note the striking differences between the two samples. Although the overall valence band width is similar, the Rutile(110) VB is broad with multiple peaks, while the Anatase(001) VB has a sharp single peak and an extended foot. There is essentially no variation of the Anatase(001) spectrum over half the Brillouin zone in the direction parallel to the surface, while the rutile(110) shows much more dispersion. The small, dispersionless state near the Fermi level on the rutile sample is a defect state about 0.4 eV below the Fermi level. It pins the Fermi level closer to the valence band maximum than in the anatase film. Both films are n-type, with the Fermi level near the conduction band minimum.