Electrical Properties of Anatase Thin Films

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Introduction

TiO_2 has been investigated extensively as a support material for catalyst particles. Most notably in recent years, anatase is preferred as a support of gold nanoparticles for oxidation of CO low temperatures. We note that there is little consideration of the composition, defect structure, or electronic properties of the anatase phase in discussing the catalytic properties, although the active gold species, the CO reaction mechanism, and the effect of the catalyst activation treatments are still not understood. There are many papers in the literature examining the electrical properties and use of anatase as a resistive gas sensor at high temperatures [1], yet at temperatures of interest for the catalytic processes and catalyst activation, there is a dearth of information. Knauth and Tuller have published conductivity studies of anatase at lower temperatures, 450-730ºC [2], although this is still far above ambient temperatures for CO oxidation reactions. Using samples fabricated as thin films, we are studying the electrical properties at 30-150ºC.

Materials and Methods

Thin films are deposited by reactive magnetron sputtering from Ti and Au targets. A variety of compositions and microstructures can be obtained by adjusting the deposition conditions. As deposited, the films are non-crystalline by x-ray diffraction, and form a polycrystalline anatase structure when annealed at 400ºC. Conductivity samples are prepared on insulating substrates with thin film metal current collectors below and above the anatase films. The films are characterized using complex impedance spectroscopy under controlled temperature and gas mixtures.

Results and Discussion

Results will be presented for pure anatase films and Au+anatase films prepared by co-deposited gold or deposition of gold particles at the surface. The films are equilibrated under different conditions of the partial oxygen pressure, reactive gas mixtures, temperature, and lighting level. In addition, we examine the rate of re-equilibration following changes in the gas mixtures. The accompanying figures show examples of the data obtained at 150ºC.

Results will be analyzed to identify the dominate lattice and electronic defects and their mobilities. These will be discussed for anatase under gas and temperature conditions typical of those used for CO oxidation and also the pretreatment activation of the powders.

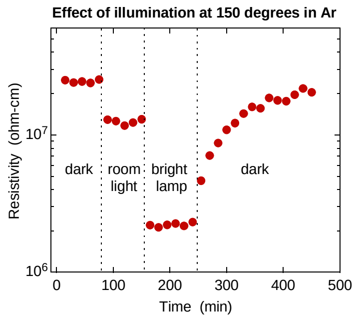

Figure 1.
Resistivity across an anatase film as the light level is varied from dark to brighter conditions and back. The film was equilibrated at 150ºC in flowing argon. Measurements are recorded for 50 Hz at 15 minute intervals.

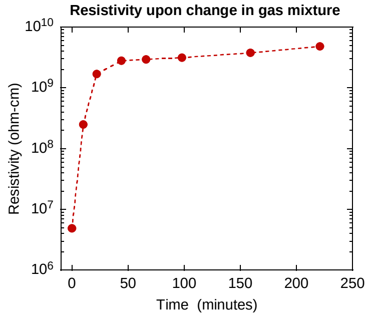

Figure 2
Resistivity across an anatase film at 150ºC during re-equilibration with the gas phase. Initially the sample was equilibrated in flowing argon, then switched to 10% O_2 in argon.

Significance

Studies of the electrical properties of anatase at low temperatures reveal the changes in stoichiometry, electronic properties, and lattice defects that may be influencing the catalysis reactions.

References

1. Fergus, J. W. *J. Mat. Sci* 38, 4259 (2003).
2. Knauth P. and Tuller, H. L. *J. Appl. Phys.* 85, 897 (1999).

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