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Defect Structure of Semiconducting and
Insulating Epitaxial Oxides

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The study of the defect structure of semiconducting and insulating epitaxial oxides has continued. During this period, the growth and characterization of epitaxial BaTiO_3 and SrTiO_3 layers were undertaken. For the growth of the epitaxial oxides, an organometallic chemical vapor deposition technique was developed. For the deposition of BaTiO_3 , we developed and used the second generation Ba precursor, barium (hexafluoroacetylacetonate)₂ (tetraglyme)($\text{Ba(hfa)}_2\cdot\text{tet}$) along with titanium tetraisopropoxide as the titanium precursor. The $\text{Ba(hfa)}_2\cdot\text{tet}$ has improved stability and volatility which is important for film composition control. While for a deposition temperature of 700°C multiphase films containing BaF_2 were deposited, at 800°C single phase BaTiO_3 layers were realized. Recently, we have succeeded in depositing epitaxial BaTiO_3 by using single crystalline LaAlO_3 substrates. This development should significantly improve our electronic property and defect structure measurements since grain boundaries are eliminated in the layers. The structure of the epitaxial BaTiO_3 was examined using both x-ray diffractometer measurements and high-resolution transmission electron microscopy (HRTEM). The x-ray diffraction $\theta - 2\theta$ scans indicated that the films had a preferred a axis orientation. In-plane epitaxy was determined from the ϕ scan data. The BaTiO_3 film and its interface with LaAlO_3 substrate were examined with HRTEM. HRTEM indicated that the films were indeed epitaxial. However, at the film/substrate interface a reaction layer of 1 nm thick was observed. Nevertheless, in some regions the interface was nearly atomically abrupt. Away

from the interface, HRTEM indicated that the films were essentially single phase, epitaxial BaTiO₃. Some areas of the films were amorphous. In collaboration with V. Dravid, EELS spectra were measured on the BaTiO₃ layers using the new Hitachi HF-2000 microscope. The detailed EELS spectra was very sensitive to the local structure of the thin film. This should yield composition/structure analysis on the nm scale.

The doping of the BaTiO₃ films has begun. Initial studies have centered on doping with the rare earth La. The undoped layers have resistivities that range from $10^2 - 10^4$ ohm-cm. The La doped layers are typically 10^2 ohm-cm. Thermopower measurements indicate that both types of layers are n-type. That the doped layers are n-type is consistent with trivalent La substituting for divalent Ba in the BaTiO₃.

To determine the electronically active defects in the BaTiO₃ thin films, deep level optical spectroscopy (DLOS) measurements have been undertaken. Here, metal-insulator-semiconductor MIS structures are used with the semiconductor in this case being silicon. DLOS measurements indicate the presence of several traps with transition energies in the range of 2.5 - 3.5 eV. Deep level transient spectroscopy measurements on the epitaxial BaTiO₃ layers are underway.

In collaboration with G. Wong, the non-linear optical properties of the BaTiO₃ thin films have been studied. Second harmonic generation has been observed; however, the efficiency so far is less than bulk BaTiO₃. Nevertheless, initial measurements on the non-linear optical properties are encouraging.

Publications

"Deposition of Ferroelectric $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ Thin Films", by L. A. Wills and B. W. Wessels, in Chemical Vapor Deposition XI, ed. by K. E. Spear (Electrochemical Soc., N.J., 1990).

"Chemical Vapor Deposited Strontium Titanate Thin Films and Their Properties", by W. A. Feil, L. M. Tonge, T. J. Marks and B. W. Wessels, *ibid.*

"Epitaxial Growth of BaTiO_3 Thin Films by Organometallic Chemical Vapor Deposition", by L. A. Wills, B. W. Wessels, D. S. Richeson and T. J. Marks, *Appl. Phys. Lett.*, in press.

" BaTiO_3 Thin Films Prepared by Organometallic Chemical Vapor Deposition", by L. A. Wills, B. W. Wessels, D. L. Schulz and T. J. Marks, in Ferroelectric Thin Films II, ed. by A. I. Kingon, E. R. Meyers and B. Tuttle, MRS, in press.

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