3.14 XPS Study of the Oxidation of Li and Ta in an Ultrahigh Vacuum Environment

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Successful deposition of thin film ferroelectric oxides requires complete in-situ oxidation. Achieving this in vacuum at relatively low growth temperatures (400-600°C) is a challenge. In order to better understand the growth of complex ternary compounds like $LiTaO_3$, we systematically studied the oxidation of the component metals, lithium and tantalum. For these experiments, tantalum or its pentoxide were deposited from an e-beam evaporator, while pure lithium was evaporated from an effusion cell. Oxygen was supplied by either a stream of molecular oxygen or oxygen activated/dissociated in an electron cyclotron resonance (ECR) plasma source. The degree of oxidation of the deposited films was investigated by x-ray photoelectron spectroscopy (XPS).

The use of molecular oxygen at tantalum deposition rates of about 0.3 Å/s led to less than 50% oxidation. When oxygen was activated in the ECR source this value increased to about 80% for the same deposition conditions. By the optimization of both the growth rate and the sample temperature we obtained fully in-situ oxidized films. The use of tantalum pentoxide as a precursor resulted in 97% oxidized films. The observed oxygen deficiency arose due to partial decomposition of the precursor during the evaporation process, but was easily compensated by the use of the ECR source. The latter process resulted in stoichiometric Ta_2O_5 thin films even at deposition rates as high as 1.3 Å/s.

The use of the ECR source in the oxidation of lithium yielded completely oxidized films in the LiO (72%) and Li_2O forms. All films showed a polycrystalline phase at substrate temperatures of 500-650 °C.