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Correlations Between XAS and Spectroscopic Ellipsometry Studies and Ab-Initio Quantum Calculations on RPE-MOCVD Deposited Titanium Silicate Alloys NICHOLAS STOUTE, GERALD LUCOVSKY, DAVID ASPNES, North Carolina State University — We report thin film titanium silicate alloys, with a range of compositions between 0 and 100% TiO_2 , deposited on Si(100) substrates through Remote Plasma Enhanced Metal Organic Chemical Vapor Deposition (RPE-MOCVD). Samples were measured in both their as-deposited condition and after a range of annealing temperatures. The conduction-band electronic structure of these alloys were analyzed through O K_1 and Ti $L_{2,3}$ X-Ray Absorption Spectroscopy (XAS) measurements as well as Spectroscopic Ellipsometry measurements performed in the 1.5 to 6 and 4.5 to 8.5 eV energy ranges. Results were correlated with previous theoretical and experimental studies as well as new Ab-Initio quantum calculations. Emphasis is placed on correlating spectroscopic data with calculations on 4-fold coordinated tetrahedral as well as 6-fold coordinated rutile and anatase structures to obtain spectroscopic signatures of phase changes and crystallization. Investigations into the effect of bond distortions on the electronic structure will also be presented.

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