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The effect of oxygen vacancies and strain on the optical bandgap of strained $SrTiO_3$ thin films NATHAN STEINLE, BARRY KOEHNE, Undergraduate Research Assisstant, RYAN COTTIER, Postdoc, DANIEL CURRIE, Postgrad, NIKOLETA THEODOROPOULOU, Research Advisor — $SrTiO_3$ (STO) films were grown on single crystal $SrTiO_3$ p-Si (001) substrates using molecular beam epitaxy (MBE). The single-phase STO/Si films were of high crystalline quality as verified by x-ray diffraction (XRD) and atomic force microscopy (AFM) with an rms roughness of less than 0.5 nm. Oxygen vacancies were introduced by controlling the oxygen pressure (varied from 10^{-8} to10^{-7} torr) during growth. Both thickness variation and oxygen pressure alter the crystal structure and electronic properties of STO. The lattice mismatch of STO on Si causes a 1.7% bi-axial, compressive strain. The oxygen vacancies cause a tensile strain because of the different Ti^{3+} and Ti^{4+} ionic radii. This agrees with our XRD measurements that show a decrease of the out of plane lattice constant as either the thickness or the oxygen pressure during growth increases. We used a Variable Angle Spectroscopic Ellipsometer M-2000 by Woolam and the VASE software to measure and model the optical properties of the films using Tauc-Lorentz oscillators for the STO layer and directly measured optical properties of Si and STO substrates. Our results show that the indirect bandgap of STO decreases as either the thickness increases or the oxygen vacancies decrease, in agreement with theoretical calculations. [1]

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