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The effect of oxygen vacancies and strain on the optical energy gap of strained $SrTiO_{3-\delta}$ thin films[1] NATHAN STEINLE, BARRY KOEHNE, Undergraduate Assisstant, RYAN COTTIER, Post-Doctoral, DANIEL CURRIE, Post-Graduate, NIKOLETA THEODOROPOULOU, Advisor — $SrTiO_{3-\delta}$ (STO) films were grown on single crystal $SrTiO_3$ and 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 ($P(O_2)$: 10^{-8} to 10^{-7} torr) during growth. 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 $P(O_2)$ during growth increase. 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 and substrates using Tauc-Lorentz and Gaussian oscillators for the STO layer. Our results show that the direct energy bandgap of STO at around 3.8 eV increases as either the thickness or $P(O_2)$ decrease, in agreement with theoretical calculations. Additionally, absorption is observed in the 1.5-2 eV region for the films with increased Oxygen vacancies.

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Nathan Steinle
Undergraduate Assisstant

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