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Hydrogen-Related Defects in Strontium Titanate[1] MARIANNE TARUN, MATTHEW MCCLUSKEY, Department of Physics and Astronomy, Washington State University, Pullman, Wa, 99164-2814 — Due to the presence of hydrogen in most as-grown crystals and their influence on the structural and electronic properties useful for device applications, efforts have been made to study hydrogen as an impurity in important compounds such as strontium titanate ($SrTiO_3$). Hydrogen forms a strong bond with oxygen, providing a powerful driving force for its incorporation in $SrTiO_3$. The resulting O-H bond gives rise to defects in $SrTiO_3$. Local vibrational modes (LVMs) of these O-H complexes are identified using IR absorption spectroscopy. Two O-H modes at 3355 and 3384 cm^{-1} wavenumbers are observed after hydrogenation at 800°C in sealed ampoules filled with H_2 gas. Isotope substitution experiments reveal that the defect consists of 2 H atoms. The thermal stability of the defect is determined through a series of isochronal annealing experiments. The observed LVMs are tentatively ascribed to a defect consisting of a Sr vacancy and 2 H atoms, each of which is bound to an O atom. This model explains the observed temperature dependent behavior of the frequency of the LVMs.

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