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Effect of elastic strain on the band gaps, band alignment, and electronic structure of epitaxial ASnO_3 ($A = \text{Ca}, \text{Sr}, \text{and Ba}$) films and heterostructures revealed through in situ photoemission, spectroscopic ellipsometry, and density functional theory JOHN BANIECKI, TAKASHI YAMAZAKI, HIROYUKI ASO, YOSHIHIKO IMANAKA, Fujitsu Laboratories, DAN RICINSCHI, Tokyo Institute of Technology — The alkaline earth stannates ASnO_3 ($A = \text{Ba}, \text{Sr}, \text{and Ca}$) are emerging as important materials. Band gaps in stannates are remarkably dependent on volumetric strain with a decrease in volumetric strain of 3 percent in SrSnO_3 resulting in an increase in the band gap of 0.35 eV. However, little understanding of volumetric strain dependence on the valence band (VB) electronic structure and band alignments between stannates and other oxides exists. In this talk we will examine the effect of elastic strain on the band gaps, band alignment, and electronic structure of stannate films and heterostructures through in situ photoemission, spectroscopic ellipsometry, scanning transmission electron microscopy with geometric phase analysis, and density functional theory. CaSnO_3 (CSO), SrSnO_3 (SSO) and La-doped BaSnO_3 (BLSO) thin films were grown by pulsed laser epitaxy with strain control via epitaxial buffer layers. While the VB electronic structure is strain dependent VB offsets do not vary significantly with strain, which resulted in ascribing most of the difference in band alignment to the conduction band (CB) edge. Significantly, strain-induced tuning of CB offset differences are as large as 0.6 eV for SSO and may provide a pathway to enhance stannate-based devices.

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