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Linking the Electronic and Atomic Structure of Epitaxial Complex Oxides on Semiconductors DIVINE KUMAH, JAMES REINER, JOSEPH NGAI, YARON SEGAL, ALEXIE KOLPAK, DIANA QIU, SOHRAB ISMAIL-BEIGI, CHARLES AHN, FRED WALKER, Department of Applied Physics, Yale University, DONG SU, YI ZHU, Brookhaven National Laboratory, ZHAN ZHANG, Argonne National Laboratory — Understanding the interfacial coupling between materials with different electronic properties is critical to achieve the integration of epitaxial complex oxides with semiconductors. Using a combination of synchrotron x-ray diffraction and first principles calculations, we show that the electronic properties and atomic structure of epitaxial $SrTiO_3$ films on Si, and $BaTiO_3$ films on Ge are directly linked to the chemical composition at their respective interfaces. Sub-angstrom [001] cation-anion displacements observed in the $SrTiO_3$/Si system, lead to a positively polarized film. The polar distortions are found to arise from an interplay between compressive strain and localized interface states. In contrast to $SrTiO_3$/Si, we find that the $BaTiO_3$/Ge interface has a 2x1 structure that drives an in-plane polarization.

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