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Understanding the atomic structure of epitaxial $SrTiO_3$-GaAs (001) hetero-interfaces. ROBERT KLIE, YIMEI ZHU, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton NY 11021, YONG LIANG, Motorola Labs, Tempe, AZ 85284, ERIC ALTMAN, Department of Chemical Engineering, Yale University, New Haven, CT 06520, WERONIKA WALKOSZ, JUAN-CARLOS IDROBO, SERDAR OGUT, Department of Physics, University of Illinois at Chicago, Chicago IL 60607 — The combination of high-resolution Z-contrast imaging, electron energy-loss spectroscopy (EELS), and density functional theory (DFT) calculations was used to study the interfacial structure of ultra-thin $SrTiO_3$ films on GaAs(001). Z-contrast imaging suggests an atomically sharp hetero-interface with $SrTiO_3$ [110] in registry with As-terminated GaAs [100] with no visible reconstruction of either surface. Our initial DFT-calculations reveal that such a stoichiometric interface would have states in the band gap, while X-ray photoelectron spectroscopy (XPS) shows a clean band gap and a valence band offset more than twice of the calculated offset. Therefore, we will use atomic-column resolved EELS and further DFT-calculations to explore the role of oxygen vacancies at the interface in compensating for the As dangling bonds and search for the low-energy semi-conducting $SrTiO_3$/GaAs-system.

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