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Structural, chemical and electronic changes at $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces near the critical thickness ROHAN MISHRA, S.T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory, JAUME GAZQUEZ, G. HERRANZ, M. STENGEL, M. SCIGAJ, N. DIX, F. SANCHEZ, J. FONTCUBERTA, Institut de Ciència de Materials de Barcelona, M. VARELA, Oak Ridge National Laboratory, Universidad Complutense de Madrid, A.Y. BORISEVICH, Oak Ridge National Laboratory — The formation of two-dimensional electron gas (2DEG) at the n-type $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) heterostructure is a paradigmatic example for emergent functionalities at oxide heterointerfaces. However, the origin of this 2DEG at the LAO/STO interface still remains unclear. In this work, we use scanning transmission electron microscopy and electron energy loss spectroscopy (STEM/EELS) to study a series of $(\text{LAO})_n/(\text{STO})$ films, both below ($n=3$) and above ($n=5,7$) the critical thickness for the formation of the 2DEG ($n>3$). From STEM imaging, we observe dramatic changes in the polar distortion of the AlO_2 layers in response to the built-in electrostatic potential in the three films. We also observe changes in the octahedral tilts across the interface for different LAO thicknesses. We obtain information about cation intermixing across the heterointerface from EELS. We combine these results with density functional theory calculations to discuss the effect of each of these different structural and chemical changes on the electronic property of the interfaces. Overall, our results present a detailed understanding of the role of electronic and atomic reconstructions and defects on the emergence of 2DEG at these interfaces.

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