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Conductivity and local structure in LaNiO_3 JENNIFER FOWLIE, MARTA GIBERT, DQMP, University of Geneva, GIULIO TIERI, DQMP, University of Geneva and LPS, Universit Paris-Sud, ALEXANDRE GLOTER, LPS, Universit Paris-Sud, JORGE IGUEZ, Luxembourg Institute of Science and Technology, ALESSIO FILIPPETTI, Istituto dei Materiali, CNR-IOM and Dipartimento di Fisica, Universit di Cagliari, SARA CATALANO, STEFANO GARIGLIO, DQMP, University of Geneva, ODILE STPHAN, LPS, Universit Paris-Sud, JEAN-MARC TRISCONE, DQMP, University of Geneva — In this study we approach the thickness-dependence of the properties of LaNiO_3 films along multiple, complementary avenues: sophisticated ab initio calculations, scanning transmission electron microscopy and electronic transport. Specifically, we find an unexpected maximum in conductivity in films of thickness 6 - 10 unit cells (3 nm) for several series of LaNiO_3 films. Ab initio transport based on the detailed crystal structure also reveals a maximum in conductivity at the same thickness. In agreement with the structure obtained from scanning transmission electron microscopy (STEM), our simulated structures reveal that the substrate- and surface-induced distortions lead to three types of local structure (heterointerface, interior-layer, surface). Based on this observation, a 3-element parallel conductor model neatly reproduces the trend of conductivity with thickness. This study addresses the question of how structural distortions at the atomic scale evolve in a thin film under the influence of the substrate and the surface. This topic is key to the understanding of the physics of heterostructures and the design of functional oxides.

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