Resolving the polar interface in superconducting nickelate thin films

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Superconducting infinite-layer nickelates [1] were first predicated as a potential analogue to the high-Tc cuprates, though some key distinctions have emerged [2]. Notably, nickelates are the most polar layered oxide superconductor yet discovered, with +/-3 formally charged atomic planes. Thus far, superconductivity has only been stabilized in epitaxial thin films, further compounding this inherent polarity with a large polar discontinuity at the atomic interface. This interface presents important questions for understanding the phenomena observed in these films: for example, it was been predicted that an ideal interface between NdNiO2 and SrTiO3 may host a high-mobility two-dimensional electron gas (2DEG) [3]. Providing access to buried interfaces with high spatial and energy resolution, scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) can probe such effects with structural and chemical sensitivity. Elemental mapping reveals a single intermediate Nd(Ti,Ni)O3 atomic layer between the substrate and film. To more completely resolve the full interface structure, we combine precise experimental analysis and density functional theory with Hubbard U term (DFT+U) calculations. Together, the combination of atomic-resolution STEM-EELS and DFT+U calculations disentangle the contributions of various structural effects at this unique, strongly polar interface for alleviating the polar discontinuity [4].

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[3] Geisler and Pentcheva. Physical Review B 102, 020502 (2020).
[4] Goodge, et al. Nature Materials 22, 466-473 (2023).