MIP: PARADIM at Cornell University, DMR-2039380 External User Project - 2024

Is Hydrogen Essential for Superconductivity in the Nickelates?

Since the discovery of high-temperature superconductivity in cuprates, work has also focused on materials with the same structures including the nickelates, as both Cu²⁺ and Ni¹⁺ have 27 electrons. The superconducting nickelates include (La,Sr)NiO₂ (equivalent to $R_{n+1}Ni_nO_{2n+2}$ with $n = \infty$ and R = La or Sr) and $R_{n+1}Ni_nO_{2n+2}$ with n = 5 and R=Nd or equivalently Nd₆Ni₅O₁₂.

Beyond superconductivity, the layered nickelates pose a synthesis challenge as a two-step fabrication process is required. An oxygenrich precursor material is first grown by traditional thin film techniques and then oxygen is removed without collapsing the structure using H_2 , NaH, or CaH₂. As these reagents contain hydrogen, the question arises whether hydrogen incorporation into the structure is a prerequisite for superconductivity.

Here, PARADIM users from Harvard and Arizona State Universities and their collaborators searched for hydrogen across a wide range of superconducting and non-superconducting layered nickelate films, with different cation and dopant chemistry, structures, growth methods, reduction conditions, and crystalline quality. They did not find significant concentrations of hydrogen in superconducting films and were also unable to use excessive reduction temperature or time to force significant amounts of hydrogen into these structures. The team's DFT calculations further corroborate that superconductivity does not rely on hydrogen.

P.P. Balakrishnan et al., Nat. Commun. 15, 7387 (2024).

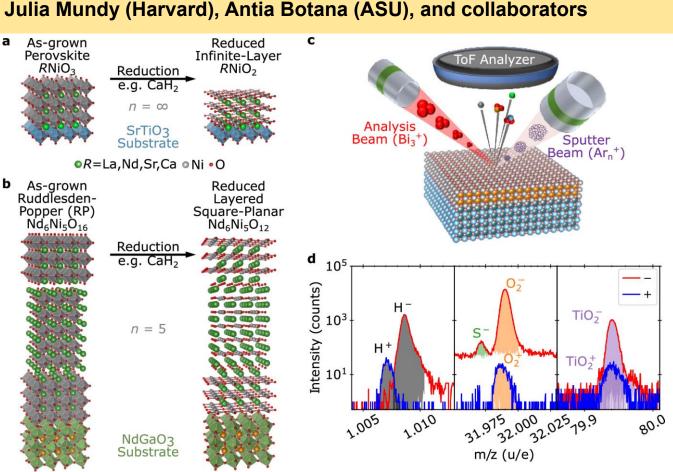


Figure: Schematic crystal structures of precursor phase and reduced to **a** $n = \infty$ and **b** n = 5 layered square-planar nickelate compounds. **c** Schematic of the ToF-SIMS measurement technique. **d** SIMS spectra measured separately for positive and negative ions are analyzed by identifying peaks by mass-to-charge ratio (*m*/*z*) and extracting integrated area.



Where Materials Begin and Society Benefits

