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Complex Oxide Interfaces: From solid-state batteries to autonomous experiments

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Metal oxides are widely used in applications ranging from energy (batteries, catalysts, etc.) to electronics (semiconductors, superconductors, dielectrics, sensors, etc.). In these applications, understanding and controlling the surfaces and interfaces of metal oxides directly affect the device performance. Therefore, it is important to clarify the electronic states and ion conduction mechanisms at the surface and interface with atomic-level spatial resolution.

Here, I first focus on solid-state batteries. Solid-state Li batteries are promising energy-storage devices owing to their high energy densities and improved safety. However, the large resistance at the interface between solid electrolytes and electrodes hinders fast charging and high-power applications.

We introduce oxide thin-film technologies for solid-state battery research. Thin-film Li batteries with controlled interfaces are ideal for detailed investigations of resistance at electrolyte-electrode interfaces because the interface area and atomic arrangements are defined.

We fabricated thin-film Li batteries with electrolyte-electrode interface resistance below ~ 5 Ω cm^2 [1,2,3,4]; this value is smaller than that observed in liquid-electrolyte-based Li-ion batteries. These studies strongly encourage solid-state Li battery research by demonstrating very low interface resistance. We also revealed that protons at the interfaces play a crucial role in determining interface resistance. Furthermore, the discussion covers the latest studies on ion-jamology [5], the interdisciplinary field of solid-state ionics and mathematical sciences.

This presentation also introduces advances in autonomous materials research [6,7]. We developed a system that automates sample handling, thin-film deposition, optimization of growth conditions, and data management (Fig. 1). Our method employs Bayesian optimization and robots to enable high-throughput experimentation, resulting in extensive datasets that cover multi-faceted properties of materials.

The system demonstrated the synthesis and optimization of electrical resistance in Nb-doped TiO_2 thin films. Moreover, this autonomous approach has discovered new ionic conductors [8]. We discuss the prospects and potential impact of this technology in accelerating materials science research, particularly in solid materials.

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