Accelerated dielectric and ferroelectric materials discovery by high-throughput thin film synthesis

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Dielectric and ferroelectric materials are fundamental to modern electronic and energy storage technologies, enabling applications ranging from high-κ gate dielectrics to capacitors and nonvolatile memories. However, the discovery and optimization of new materials through conventional trial-and-error approaches remain slow and resource-intensive. Establishing a general-purpose platform that integrates materials informatics, combinatorial synthesis, and high-throughput characterization can dramatically accelerate the exploration of complex composition-structure-property relationships. Such an approach enables rapid mapping of materials phase space, identification of promising candidates, and iterative feedback between data-driven prediction and experimental realization, ultimately transforming the pace of dielectric and ferroelectric materials innovation.

In this talk, I will discuss our progress on developing high-throughput thin film synthesis for ferroelectric and dielectric thin films. In the first part, I will discuss the design of $(Ba_{0.7}Ca_{0.3})TiO_3$ (BCT) and $Ba(Ti_{0.8}Zr_{0.2})O_3$ (BZT) superlattices via a high-throughput combinatorial approach. In the second part of the talk, I will discuss strategies to further optimize domain structures and suppress the leakage current in BZT-BCT films via a machine learning approach. The large polarization and the delayed polarization saturation led to greatly enhanced energy density of 80 J/cm^3 and transfer efficiency of 85% over a wide temperature range. Such a data-driven design recipe for a slush-like polar state is generally applicable to quickly optimize functionalities of ferroelectric materials. Figure 1 shows the schematics of the combinatorial synthesis approach of growing the BCT-BZT thin films.

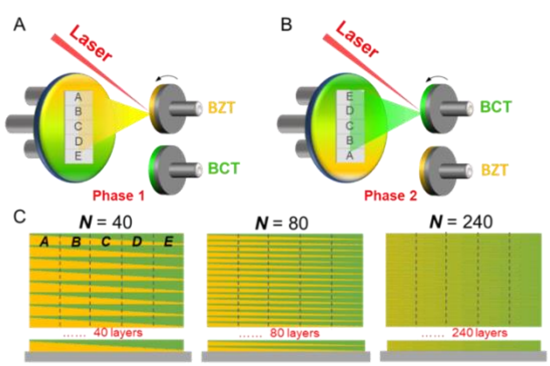

Figure 1. Combinatorial synthesis of BCT-BZT thin films. (A, B) Schematics of the combinatorial synthesis approach of growing the BCT-BZT thin films for Phase 1 and 2. (C) Schematics of the cross-sectional views of S40, S80, and S240 BCT-BZT films.

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