

## Atomic-resolution Probing of Anion Migration in Perovskites with In-situ (S)TEM

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### ABSTRACT

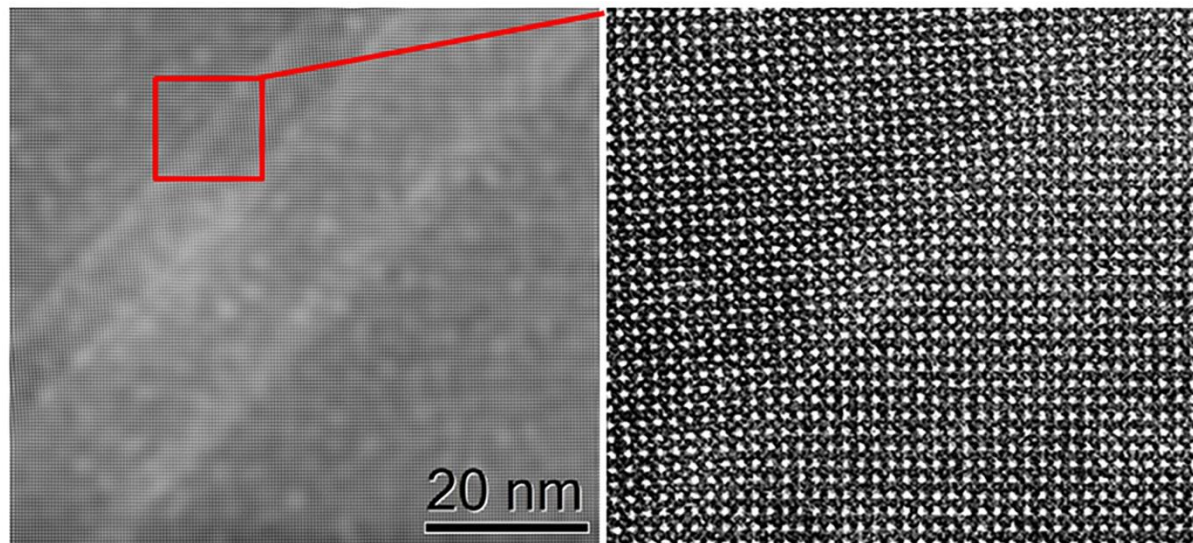
Perovskites are promising functional materials for their optoelectronic properties and anion migration plays a key role in their functional performance [1-3]. By using in-situ (S)TEM mechanical and electrical testing in conjunction with 4D-STEM [4,5], we directly observed/probed anion migration in perovskites at atomic resolution (see Figure 1). Here, we studied the mechanism for the anion migration in perovskites such as (PbZr)TiO<sub>3</sub> and BaTiO<sub>3</sub>, which is induced under the mechanical/electrical loading. To avoid the influence of the electron beam, we carried out the in-situ (S)TEM study at 60kV with low dose. And to avoid the possible strong size effect and the substrate (interface) influence, we prepared free-standing sub-micrometer single-crystalline structures to perform the experiments. Corresponding EDS and EELS examinations were performed to measure the local chemical change with applied stress and electrical currents. Our observations revealed the coexistence of multiple phase structures and hierarchical domain structures, as well as the greatly enhanced anion drifting and diffusion at the charged domain walls (Figure 2) and phase boundaries. The complex interaction between the local domain evolution and phase transition has been discussed. Based on above investigations, a model for anion migration in perovskite under mechanical/electrical loading has been presented.

### ACKNOWLEDGEMENTS

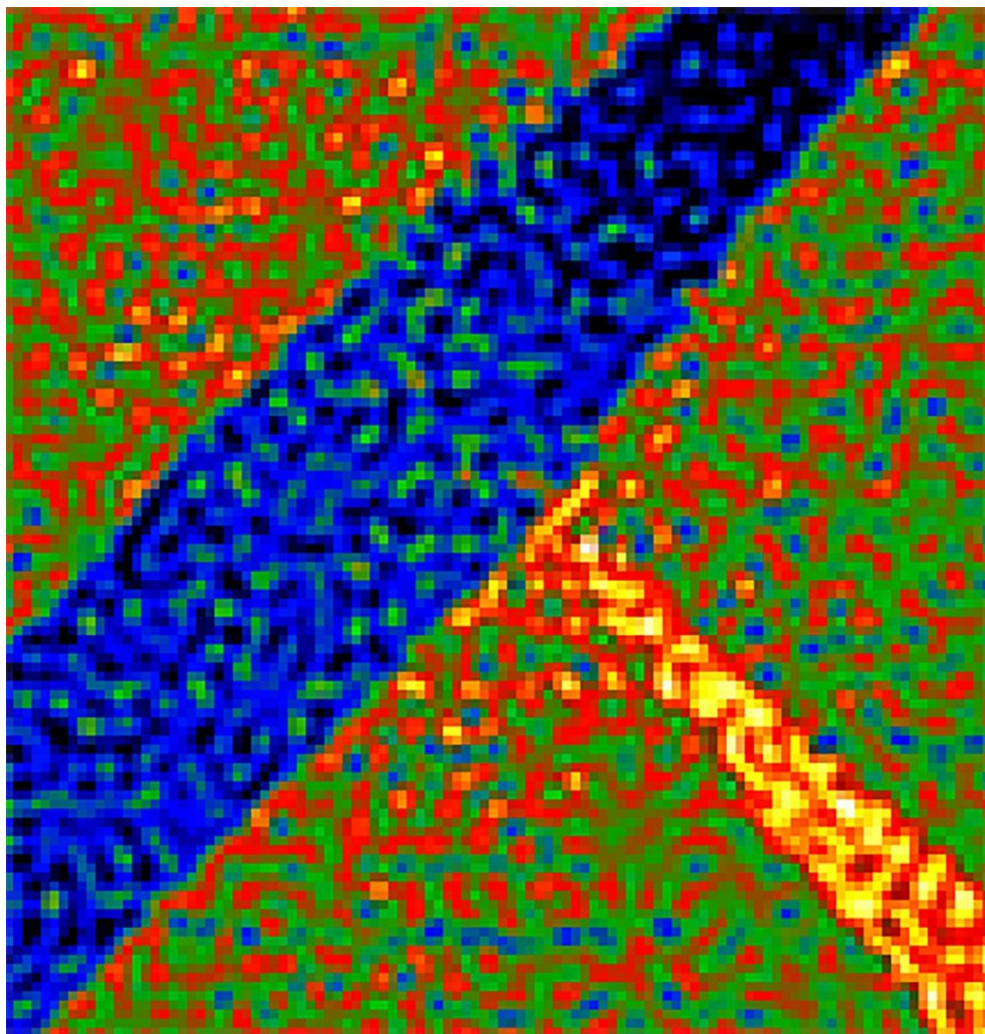
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**Figure 1.** Figure 1 The in-situ atomic-resolution observation of a (PbZr)TiO<sub>3</sub> under compression loading, where anion migration is induced at domain wall.



**Figure 2.** Figure 2 The 4D-STEM mapping on the charged domain wall in (PbZr)TiO<sub>3</sub>