Topotactic phase transformation observed in real-time in atomic-scale

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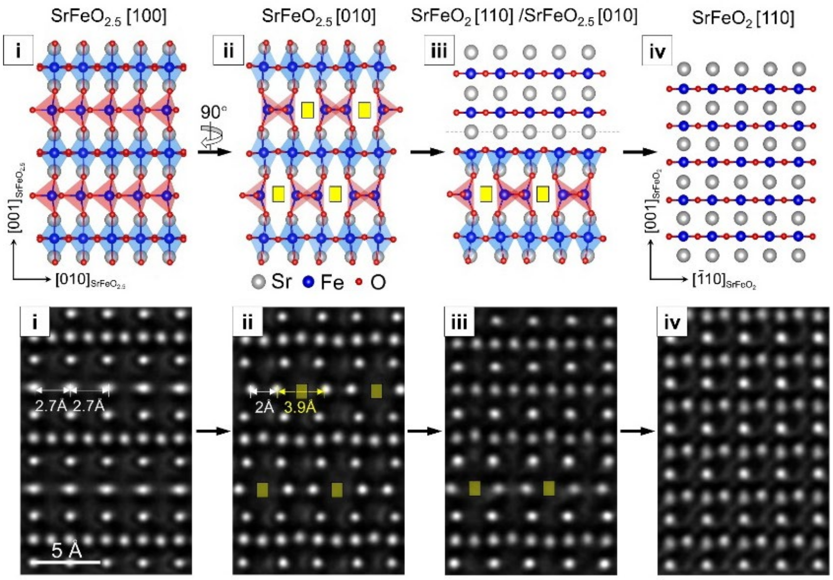
Oxygen plays an essential role in determining the materials properties of transition metal oxides. By changing the oxygen concentration only by ~30%, the electronic ground state of complex oxides may vary from insulator to metal to superconductor. Despite the general lattice structural similarity offered by the topotactic phase transformation, the change in the oxygen content necessarily accompanies the surrounding electronic environment of the transition metal – oxygen polyhedra, and the dimensionality and anisotropy of the polyhedral network. This largely modifies the electronic and phononic energy band dispersion along with the change in the apparent valence state of the transition metal ions. Hence, after the discovery, the topotactic phase transformation has been frequently employed to explore novel hidden physical properties with metastable structures. A real-time atomic-scale observation of the topotactic phase transformation, if plausible, would provide microscopic understanding of the dynamic evolution of the oxygen removal of conventional perovskite oxides, from octahedral to tetrahedral to square planar polyhedral configurations. Here, we present a prototypical example of such evolution in $SrFeO_x$ epitaxial thin films. In particular, the anisotropic brownmillerite structure promote unexpected sequential structural evolution associated with the facile movement of the oxygen within the structure. Our study would help construct a design principle in obtaining novel oxide phases with diverse transition metal – oxygen polyhedral configurations.



Real-time atomic-scale observation of the topotactic phase transformation toward infinite-layer $SrFeO_2$.

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