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Anisotropic Swelling Governed By Orientation-Dependent Interfacial Na Diffusion in Single-Crystalline

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ABSTRACT

The anisotropic volume expansion of anode materials produces locally inhomogeneous residual stresses, which frequently induce fracture of the anode materials and reduce battery capacity and cycle life. Much of our understanding of the anisotropic swelling behavior of anode materials is based on electron microscopy and macroscopic structural analysis techniques, which are insufficient to elucidate the atomistic origin of the anisotropic swelling behavior. In this study, we perform in situ sodiation experiments with single-crystalline Sb anodes followed by atomic simulations to determine the diffusion kinetics governing the sodiation of Sb and its associated swelling behavior. In situ sodiation experiments demonstrate that the diffusion rate of Na into single-crystalline Sb anodes differs by more than a factor of two depending on the orientation of the Sb crystal, causing the crystal to swell anisotropically. This observed anisotropic diffusion is explained here by determining the orientation-dependent diffusion kinetics, while the associated structural origins are clarified by studying the interfacial Na diffusion in the atomically thin layer preceding the advancing interface.

Keywords: Na-ion battery; Sb anode; anisotropic sodiation; in situ sodiation experiments; firstprinciples calculations