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Structural Changes Driven by Li Flux Density in Initial Lithiation of Single Crystal Silicon LI-QIONG WANG, MYEONGHUN SONG, SIVA NADIMPALLI, PRADEEP GUDURU, VIJAY SETHURAMAN, MICHAEL CHON, Brown University — Structural changes in amorphous Li_xSi were investigated as a function of Li flux density and total charge in the initial lithiation of single crystal (100) Si wafers using solid-state ^7Li nuclear magnetic resonance (NMR) spectroscopy. We chose a single crystal Si wafer as a model system in this study because of well-controlled Li flux density uniformly distributed across the surface of a silicon wafer. In contrast to a widely accepted $Li_{3.5}Si$ structure for the initial lithiation, this study shows a surprising finding of varying Li_xSi structures that are controlled by the Li flux density but not by the total charge. In particular, we discovered that the rate constant and the reaction mechanism at the reaction front depend on the Li flux density. The previous kinetic model is required to include the Li flux density dependent rate constant to accurately describe the reaction front kinetics in the initial lithiation of crystalline silicon. Our study provides new insight toward the understanding of the kinetics, the reaction mechanisms, and the kinetic modeling of chemical reactions at the reaction front.

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