Investigation of Facet Selective Li Deposition on Cu Current Collectors for Anode-free Lithium Metal Batteries

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Achieving a more uniform Li deposition/dissolution on a current collector is a critical step forward in achieving anode-free or low Li metal-loaded lithium metal batteries. Here, we explore a facet selective Li nucleation and growth phenomenon on Cu and demonstrate that controlling the facet structure can improve the uniformity in Li deposition and the cycling stability. Preferential Li deposition on the Cu(100) plane is demonstrated by electrochemical analysis of the Cu single crystal surfaces and by EBSD analysis of the Li-deposited Cu surfaces. DFT calculations show that a difference in the Li adsorption energy during the initial Li deposition process among the Cu facets is responsible for the facet selectivity. A majorly (100) plane-orientated Cu foil fabricated with a simple annealing method has a more uniform Li nucleation with a 6-times higher nuclei density and a two-fold enhancement in the Li cycling stability compared with a conventional Cu foil with randomly oriented surface facets. The control of the surface facet provides a new design principle for the current collector of lithium metal batteries.