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Nucleation and Growth in Electrochemically Deposited Metals

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Abstract

Electrochemical deposition of metals, such as Li, Na, K, Zn, Mg and alike, are very important for energy storage and rechargeable battery applications. Yet, the fundamental understanding of the deposition process of these metals is surprisingly overlooked and lacking. It is often observed that the deposit's morphology, microstructure, and the associated properties are often controlled by the kinetic processes that govern the evolution of these properties with time. However, the mechanism and mechanistic processes involved are difficult to characterize to yield quantitative and sufficiently detailed temporal information to help us understand the underlying principles that govern the phase lattice structural and morphological changes. Here, we applied reactive molecular dynamics (r-MD) simulation to model the nucleation and growth processes of Li metal deposition in typical electrochemical cells. Cryo-EM was used to characterize the microstructure, morphology and relevant properties of the Li metal deposits obtained from a range of current density and duration. Both cryo-TEM and r-MD results suggest that the Li deposits are likely amorphous in the initial deposition and such amorphous phase was retained more easily at lower current density such as 0.1 mA cm^{-2} than those at 1 mA cm^{-2}. The r-MD simulation explained the cause of such amorphous phase retention is due to the significantly longer phase transition time associated with the transition from the disordered amorphous phase to the ordered crystalline phase of body-centered cubic (bcc) lattice structure. Such a long incubation could be easily understood, but hardly emphasized in the literature. Therefore, this critical aspect was often overlooked in the discussion of the experimental results, where kinetic effects are dominating the processes in the observations. We registered similar observations in other electrochemical metal depositions, and this thermal-activation-inhibited incubation process is being observed in all experimental conditions disregarding which elemental metal and lattice structure involved. The implication of this fundamental understanding will be discussed in this presentation.