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Simulation of dendrite formation in lithium-ion batteries NING SUN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, NY, 11794 — The design of the next generation of energy storage technologies requires both a fundamental understanding of the physical and chemical reactions taking place in a complex electrochemical environment and the factors that limit the performance of these systems. We have developed a Lattice-Boltzmann model to simulate 2-D dendrite formation during charging and discharging processes on the anode of lithium-ion batteries. Our results show that the formation of dendrites is strongly influenced by the morphology of the anode, and operating conditions, in particular the charging current density. Our simulation is able to recover the structures that form on Li anodes, including mossy and dendritic structures as a function of parameters such as the curvature of the interface and the applied current density. We also show that we can observe a linear relationship between the log current density (J) and the log dendrite formation onset time (ts) in the low current density region, which also agrees with experiment data quite well. We study additional effects such as the role of the separator and the Solid Electrolyte Interphase (SEI) layer on the formation of dendrites.

> Ning Sun Stony Brook University

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