A Lattice Boltzmann Method Based Computational Model for Optimizing Anode Morphologies to Design Efficient Li-ion Batteries

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The study of Li-ion batteries (LIB) is critical because of their widespread application in commercial electronics and electric vehicles. Graphite, the predominant LIB anode material, fails to achieve high charge capacities and forms dendrites at high currents, resulting in safety hazards. The research created a novel Lattice Boltzmann Method (LBM) based model to simulate the LIB charging process and devised an optimal anode morphology. LBM was utilized as the framework to model the mass transfer of Li-ions while boundary conditions and reactions were governed by electrochemical principles. An algorithm was developed to generate a random morphology, resembling industrial anode structures, with additional constraints applied for the controlled morphology. The two morphologies were compared under constant current and constant potential environments. The results were validated by a 3D model and the computational efficiency of parallel processing was analyzed. At constant potentials, the controlled morphology attained 13% higher currents and charge capacities than the random morphology. At constant currents for porous systems, the controlled morphology attained 23% higher charge capacities than the random morphology at high applied currents. The results of the 2D and 3D models were equivalent. Parallelization analysis revealed that 9 and 13 processors were optimal for composite and prime cores respectively. The project created an extendable and scalable LBM model to simulate the LIB system. It provided insight into designing an optimal anode morphology, useful as a cost-effective prescreening tool for anode testing. The controlled morphology performed well for porous systems, allowing insertion of conductive and binder materials.

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