Molecular Dynamics Study on Dendrite Formation Mechanism in Li-ion Battery

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Clean energy storage has become tremendously important to overcome the challenges arise from the depleting non-renewable resources and climate change. To this end, Li-ion battery with Li anode has emerged as a promising solution, which offers theoretically high energy storage capacity. Nevertheless, it is still plagued with safety issue due to dendrite formation during charge-discharge cycle, which can cause short-circuit. In spite of many studies, the dendrite formation mechanism is still not clear. Herein, molecular dynamics (MD) simulation is used to unravel dendrite formation mechanism and intrinsic factors, which cause dendrite formation. Several factors which being investigated are different Li anode surfaces (e.g., Li(100), Li(110), Li(111), and Li(211)), electric field strength, anode surface charge, and temperature. However, continuous redox reaction occurs in battery cannot be described with classical MD alone. To further investigate this, we aim to develop custom LAMMPS code to correctly describe redox reaction and charge equilibration of Li-ion. Additionally, convex hull algorithm is used as the criteria of Li-ion deposition on Li anode.