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Simulation of Stress in Graphite Anode of Lithium-Ion Battery: Intra and Inter-Particle

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Abstract : The volume expansion of lithium-ion batteries is mainly induced by intercalation induced stress within the negative electrode, resulting in capacity degradation and even battery failure. Stress generation due to lithium intercalation into graphite particles is investigated based on an electrochemical-mechanical model in this work. The two-dimensional model presented is fully coupled, inclusive of the impacts of intercalation-induced stress, stress-induced intercalation, to evaluate the lithium concentration, stress generation, and displacement intra and inter-particle. The results show that the distribution of lithium concentration and stress exhibits an analogous pattern, which reflects the relation between lithium diffusion and stress. The results of inter-particle stress indicate that larger Von-Mises stress is displayed where the two particles are in contact with each other, and deformation at the edge of particles is also observed, predicting fracture. Additionally, the maximum inter-particle stress at the end of lithium intercalation is nearly ten times the intraparticle stress. And the maximum inter-particle displacement is increased by 24% compared to the single-particle. Finally, the effect of graphite particle arrangement on inter-particle stress is studied. It is found that inter-particle stress with tighter arrangement exhibits lower stress. This work can provide guidance for predicting the intra and inter-particle stress to take measures to avoid cracking of electrode material.

Keywords : electrochemical-mechanical model, graphite particle, lithium concentration, lithium ion battery, stress
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