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Modeling Sodium-Ion Electrode Manufacturing via the Lattice-Particle Method: From Slurry Drying to Calendering

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Abstract

The global shift toward sustainable energy has accelerated the development of sodium-ion batteries (NIBs) as a cost-effective and abundant alternative to lithium-ion technologies. However, the industrial scale-up of NIBs requires a deep understanding of the manufacturing chain, where the transition from a wet slurry to a functional electrode significantly dictates final performance. While the Discrete Element Method (DEM) is commonly used to model these processes, its high computational cost and calibration complexity often limit its application in real-time manufacturing optimization. This work presents a novel, computationally efficient digital twin framework based on the Lattice-Particle Method (LPM) to simulate the manufacturing of NIB electrodes. The proposed approach bridges two critical, interconnected stages: slurry drying and calendering. Unlike traditional models that treat these steps in isolation, our framework utilizes a seamless LPM architecture where the electrode components (e.g. active particles, additives) are represented within a network of one-dimensional elements. The simulation begins with the drying stage, solving a coupled thermomechanical problem that accounts for the material shrinkage. This step determines the initial heterogeneous microstructure. Subsequently, the model transitions into the calendering stage, where the mechanical compaction is solved using a constitutive relationship based on the Johnson, Kendall, and Roberts (JKR) contact model. By integrating these steps, we capture the evolution of the electrode's porosity, connectivity, and

mechanical integrity from its initial liquid-like state to its final densified form. The results demonstrate that the LPM framework can effectively predict microstructural features such as tortuosity and pore distribution at a fraction of the computational cost of traditional DEM. Moreover, it represents the foundation of a potential digital twin of the NIB production line, enabling the virtual optimization of processing parameters to enhance the electrochemical performance of next-generation batteries.

Keywords:

lattice-particle electrode calendering slurry drying Na-ion batteries