Tech Science Press

ICCES, 2024, vol.30, no.3
DOI: 10.32604/icces.2024.012815

PROCEEDINGS

Three-Dimensional Discrete Element Simulation of Electrode Structural Evolutions in Lithium-Ion Batteries During Drying and Calendering

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ABSTRACT

Drying and calendering processes are crucial in electrode manufacturing, as they significantly affect the mechanical and electrochemical performances of lithium-ion batteries. In this study, we established a three-dimensional (3D) representative volume element (RVE) of electrodes composed of active material particles, carbon binder domain particles, solvent, and different particle contact types. We continuously simulated the 3D macroscopic and microscopic structural evolutions of the RVE during drying and calendering using the discrete element method (DEM). Based on the evolution of the particle coordination numbers and contact networks during drying, we propose a three-stage-drying scheme, consistent with the relevant experimental results. Analyses of the evolution of porosity, particle coordination number, and contact network of the RVE show that the mechanical integrity and electronic conductivity of the electrodes can be significantly improved by calendering. The stress acting on the electrode particles is in a 3D compression state during calendering, and the maximum stress appears along the thickness dimension of the electrodes. Thus, this study demonstrated the significant potential of DEM in the study of electrode heterogeneity during drying and calendering processes.

KEYWORDS

Discrete element method; electrode slurry; drying; calendering; structural evolution; representative volume element

Acknowledgments: The authors gratefully acknowledge the financial support of the National Natural Science Foundation of China (Nos. 12172206 and 11972218).

Declaration of competing interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.