

PROCEEDINGS

Spatiotemporal Dynamics of Multiple Side Reactions and Thermal Runaway in Lithium-Ion Batteries Under High-Temperature Abuse

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ABSTRACT

The vulnerability of lithium-ion batteries to thermal runaway under abuse conditions, particularly high temperatures, remains a critical bottleneck for their widespread deployment [1-6]. Here, we present a three-dimensional electro-thermo-chemical multiphysics model to elucidate the complete spatiotemporal evolution of thermal runaway under thermal oven tests. By seamlessly integrating solid-state heat transfer with Arrhenius reaction kinetics, our framework rigorously resolves the three primary exothermic side reactions: solid electrolyte interphase (SEI) decomposition, anode-solvent interaction, and cathode breakdown. Our results reveal that the thermal response of the battery during oven exposure is characterized by three distinct phases: external heating, exothermic heat accumulation, and explosive thermal runaway. The simulations explicitly decode the underlying chain-reaction mechanism: at ~25 min, SEI decomposition acts as the initial trigger; this is followed by sustained anode reactions that progressively accumulate heat, yielding a gradual temperature plateau near 150 °C. Ultimately, at ~116 min, violent cathode decomposition yields an acute spike in heat generation, driving an instantaneous temperature surge to a peak of 212.2 °C. Furthermore, we formulate a preliminary simulation framework for mechanical nail penetration based on internal short-circuit (ISC) mechanisms. This lays the theoretical groundwork for future studies to comparatively dissect "outside-in" versus "inside-out" thermal runaway pathways.

KEYWORDS

Lithium-ion batteries; thermal runaway; multiphysics simulation; side-reaction kinetics; oven test

Acknowledgement: We gratefully acknowledge the support from the National Natural Science Foundation of China.

Funding Statement: This work was sponsored by NSFC (92160203, 12172035).

Conflicts of Interest: The authors declare no conflicts of interest to report regarding the present study.

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