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Integrated computation model of lithium-ion battery subject to nail penetration

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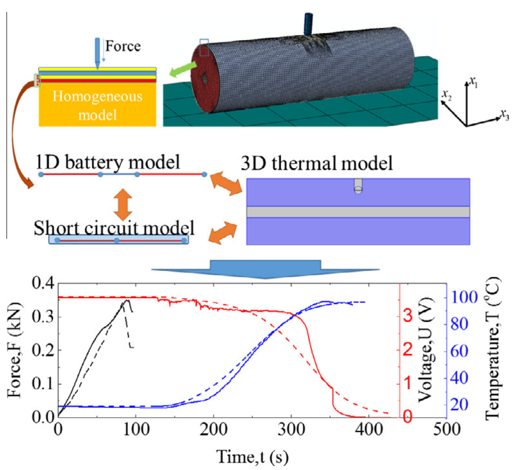
HIGHLIGHTS

- A coupling model to predict battery penetration process is established.
- Penetration test is designed and validates the computational model.
- Governing factors of the penetration induced short-circuit is discussed.
- Critical safety battery design guidance is suggested.

GRAPHICAL ABSTRACT



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ABSTRACT

The nail penetration of lithium-ion batteries (LIBs) has become a standard battery safety evaluation method to mimic the potential penetration of a foreign object into LIB, which can lead to internal short circuit with catastrophic consequences, such as thermal runaway, fire, and explosion. To provide a safe, time-efficient, and cost-effective method for studying the nail penetration problem, an integrated computational method that considers the mechanical, electrochemical, and thermal behaviors of the jellyroll was developed using a coupled 3D mechanical model, a 1D battery model, and a short circuit model. The integrated model, along with the sub-models, was validated to agree reasonably well with experimental test data. In addition, a comprehensive quantitative analysis of governing factors, e.g., shapes, sizes, and displacements of nails, states of charge, and penetration speeds, was conducted. The proposed computational framework for LIB nail penetration was first introduced. This framework can provide an accurate prediction of the time history profile of battery voltage, temperature, and mechanical behavior. The factors that affected the behavior of the jellyroll under nail penetration were discussed systematically. Results provide a solid foundation for future in-depth studies on LIB nail penetration mechanisms and safety design.

1. Introduction

The sales of electrical vehicles (EVs) have increased in the last few years [1], and lithium-ion batteries (LIBs) have been regarded

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Nomenclature

C	heat capacity
c	concentration
D_{eff}	modified diffusion coefficient
d	displacement
d_{fl}	separator failure displacement
d_{pn}	penetration displacement
$d_{pn}(t)$	penetration displacement with time
E	Young's modulus
E_p	in-plane modulus
E_t	transverse modulus
E_{tg}	tangent modulus
E_J	joule heating energy
E_{eq}	equilibrium potential
F	Faraday's constant
G_p	shear moduli in in-plane directions
G_t	shear moduli in transverse directions
H	height
I	current
I_{st}	stable current
$\underset{\rightarrow}{i}$	current density
j	current density
k	thermal conductivity
k_a	thermal conductivity in angular direction
k_r	thermal conductivity in radial direction
L	length
N	number
q_a	reaction heat
q_j	joule heat
q_r	resistance heat
q_i	irreversible heat
q	heat generation rate
R	radius
R_g	gas constant
R_r	resistance
S	area
SOC	state of charge value
T	temperature
t	time
t_c	current increasing time
t_+	transfer data
V	voltage
v_{pn}	penetration speed
δ	thickness
ϵ	volume fraction
ε	strain
ε_i $(i = 1, 2, 3)$	principle strain
ε_p	plastic strain
ε_{pc}	critical plastic strain
$\bar{\varepsilon}_f$	failure strain
$\dot{\varepsilon}$	strain rate
$^*\dot{\varepsilon}$	dimensionless plastic strain rate of winding nail
ε_{ik} and γ_{ik} $(i = 1, 2, 3;\ k = 1, 2, 3)$	strains in different directions
κ	electrical conductivity
κ_{eff}	modified electrical conductivity
v	Poisson's ratio
v_{pt}	Poisson's ratio in in plane–transverse directions
v_{tp}	Poisson's ratio in transverse–in plane directions of the jellyroll
ρ	density
σ	stress
σ_{Hill}	Hill'48 equivalent stress
σ_{ik} and τ_{ik} $(i = 1, 2, 3;\ k = 1, 2, 3)$	stresses in different directions
σ_{Mises}	von Mises equivalent stress
σ_0	yield stress
ϕ	potential
$1 + \frac{d \ln f}{d \ln c_l}$	molar activity coefficient

Subscripts

eff	modified
eq	equilibrium

Superscripts

a	anode
c	cathode
D	diffusion
j	jellyroll
l	electrolyte
nc	negative collector
ng	negative electrode
nl	penetration nail
pc	positive collector
ps	positive electrode
s	electrode
se	separator
st	short circuit part
w	winding nail
3D	3D thermal model

as promising alternative energy sources for use in EVs [2,3]. LIB safety has become one of the main topics with regard to passenger safety because LIBs are frequently used in vehicles [4,5]. A thermal management system (TEM) is generally used to prevent overheating [6–8], but a short circuit may produce a significant amount heat that may cause thermal runaway [9].

Nail penetration, which mimics the penetration of foreign objects into LIB during use, has become a standard LIB safety evaluation method [10]. The immediate consequences of nail penetration include the occurrence of internal short circuit, which has potentially catastrophic consequences, such as fire and explosion [11–13]. In general, engineers must perform time-consuming and hazardous nail penetration tests [10,14]. These tests involve inserting a steel nail into LIB, thereby bridging the positive and negative electrodes within the jellyroll and causing local internal short circuit among the component interfaces of the nail and the jellyroll. Although nail penetration is essentially a mechanical loading process, it may involve electrochemical and thermal behaviors, which result from the strong entanglement of the multiphysical fields within the battery. Thus, a reasonable modeling framework is urgently required to understand and control the complicated mechanisms of a nail penetration-induced thermal runaway or fire.

Numerical modeling is an ideal substitution for real-world nail penetration testing. First, pioneering efforts have been made to understand the mechanical behavior of LIBs that are subjected to physical abuses, e.g., radial compression [15,16], indentation [15,17], and bending [15] loads. The constitutive model for the jellyroll was first established by Greve and Fehrenbach [15] and Sahraei et al. [18] through homogeneous isotropic material treatment. Since then, Lai et al. [16] developed a representative volume element (RVE) model that considered each component of the jellyroll. Recently, an anisotropic model with coupled strain rate and state of charge (SOC) dependencies was proposed in Ref. [19]. Second, with regard to electrochemical behavior, a 1D battery model was