

Experimental Investigation of Nail Penetration-Induced Thermal Runaway and Particulate Emissions in NMC Lithium-Ion Batteries

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

Lithium-ion batteries (LIBs) have become a prominent energy storage technology for electric vehicles (EVs), consumer electronics, and stationary energy storage systems due to their high energy density and long cycle life. The growing demand for clean transportation and energy storage has accelerated their widespread adoption. However, this rapid growth has also heightened concerns regarding thermal runaway (TR), a hazardous failure phenomenon in LIBs capable of producing fires, explosions, and the release of toxic gaseous and particulate emissions. Among the abuse tests used to investigate LIB safety, nail penetration (NP) testing is widely employed to simulate mechanically induced internal short circuits (ISCs) within the cell. Despite extensive research, the influence of operating conditions on NP-induced TR behaviour and the characteristics of particulate emissions generated during failure remain insufficiently understood.

This thesis experimentally investigates the influence of state-of-charge (SOC) and low-temperature preconditioning on NP-induced TR behaviour of commercially available LG-HG2 (INR18650HG2) LIB cells. Temperature measurements and visual observations were used to evaluate ignition behaviour, thermal response, combustion characteristics, and test repeatability. The TR behaviour of commercially available LIBs with different chemistries and form factors was also compared. Finally, particulate matter (PM) generated during NP-induced TR was characterized using particle size distribution (PSD) analysis, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD).

The experimental results demonstrated a strong dependence of TR severity on SOC. Cells tested at 100%, 95%, and 77% SOC underwent immediate TR following NP, whereas the 68% SOC cell did not ignite and exhibited only sustained venting and smoke generation. Low-temperature preconditioning reduced the severity of TR, producing lower peak temperatures and, at $-40\text{ }^{\circ}\text{C}$, delayed ignition in multiple experiments. Comparative testing further demonstrated distinct differences in ignition behaviour, venting characteristics, and combustion response among cells with different chemistries and form factors, emphasizing the influence of battery design on failure behaviour.

Post-mortem characterization of TR ejecta revealed that the emitted PM consisted predominantly of submicron particles with spherical, irregular, agglomerated, and flake-like morphologies. SEM-EDX analysis identified carbon-rich particles together with metallic species originating from battery components, while XRD analysis confirmed the presence of crystalline decomposition products associated with cathode materials. These findings contribute to a more comprehensive understanding of NP-induced TR and particulate emissions from LIBs, providing valuable information for battery safety assessment, failure modelling, and the development of safer battery technologies.

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List of Abbreviations

Abbreviation Definition

AAS	Atomic Absorption Spectroscopy
ARC	Accelerating Rate Calorimeter
ATR-FTIR	Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy
BEV	Battery Electric Vehicle
BESS	Battery Energy Storage System
BMS	Battery Management System
CC-CV	Constant Current–Constant Voltage
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
DEC	Diethyl Carbonate
DMC	Dimethyl Carbonate
ECD	Equivalent Circular Diameter
EDS	Energy Dispersive Spectroscopy
EDX	Energy Dispersive X-ray Spectroscopy
ELPI+	Electrical Low-Pressure Impactor Plus
EMC	Ethyl Methyl Carbonate
EV	Electric Vehicle
FAA	Federal Aviation Administration
FESEM	Field Emission Scanning Electron Microscope
FTIR	Fourier Transform Infrared Spectroscopy
GC	Gas Chromatography
GC-MS	Gas Chromatography–Mass Spectrometry
GHG	Greenhouse Gas
HF	Hydrofluoric Acid
ICP-OES	Inductively Coupled Plasma Optical Emission Spectroscopy
LIB	Lithium-Ion Battery

Abbreviation Definition

LCO	Lithium Cobalt Oxide
LFP	Lithium Iron Phosphate
LTO	Lithium Titanate Oxide
MFA	Methoxy Formic Acid
NCA	Lithium Nickel Cobalt Aluminum Oxide
NMC	Lithium Nickel Manganese Cobalt Oxide
NP	Nail Penetration
PM	Particulate Matter
PPE	Personal Protective Equipment
PSD	Particle Size Distribution
PTFE	Polytetrafluoroethylene
SEM	Scanning Electron Microscopy
SEI	Solid Electrolyte Interphase
SOC	State of Charge
TA	Thermal Abuse
TC	Thermocouple
T_{ej}	Ejecta Temperature
T_{em}	Chamber Ambient Temperature
TR	Thermal Runaway
T_s	Battery Surface Temperature
VOC	Volatile Organic Compound
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction
ZEV	Zero Emission Vehicle

Chapter 1 Introduction

1.1 Overview and Motivation

The transport sector emits significant amounts of greenhouse gases. For example, in 2023, the transport sector accounted for 23% of Canada's total GHG emissions, which was one percentage point higher than the previous year [1]. Globally, transport remains a major contributor to GHG emissions: in 2024, the transport sector emitted about 8.4 Gt CO₂-equivalent, representing roughly 15.9% of total global GHG emissions [2]. Therefore, the past decade has seen a significant rise in the global effort to transition towards cleaner energy systems within the transport sector [3], [4], [5], [6]. For example, Transport Canada has set a goal of achieving net-zero emissions by 2050, which is highlighted in the 2030 Emissions Reduction Plan. The Canadian government also has a mandate that requires 100% zero-emission light-duty vehicle sales by 2035 [4]. Globally, many other countries and regions have set similar deadlines. The International Energy Agency (IEA) notes that in its "net-zero" scenario, light-duty vehicle sales worldwide, including cars and vans, are projected to become fully zero-emission by 2035 [5]. These global efforts have led to a rapid expansion of electric vehicles (EVs) within the transportation sector [6]. For instance, in 2023, Canada's zero emission vehicle (ZEV) market share reached 11.7%, a significant increase from 3.1% in 2019. The ZEVs, encompassing both battery electric vehicles (BEVs) and plug-in hybrid electric vehicles, saw sales exceeding 15% by the third quarter of 2024 in Canada [7]. By the second quarter of 2024, the adoption rate of BEVs alone in Canada hit 12.2% [8].

Among all the rechargeable batteries, lithium-ion batteries (LIBs) are favored in EVs for their high energy density and extended shelf life [9] , [10]. Compared to lead-acid or nickel-metal hydride batteries, LIBs have a higher cathode potential, and hence, higher energy density, and they also have greater cycle life, as shown in **Figure 1 (a)** [11]. Moreover, LIBs possess a high power-to-weight ratio, improved thermal stability, and a low self-discharge rate [12], [13], [14], [15].

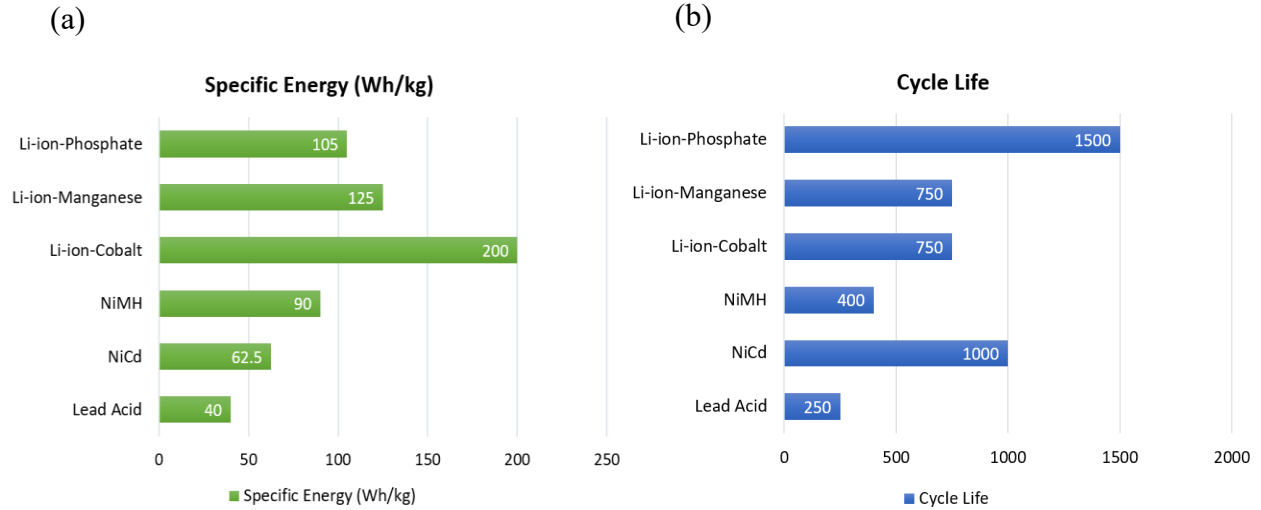


Figure 1: Specific energy (a) and cycle life (b) comparison between LIBs and other secondary cells. Recreated originally from [11]

As a result, LIB demand has risen, and its use has become widespread. For example, in 2023, the sales of EVs accounted for 95% of the increase in global LIB demand, totaling over 750 Gigawatt-hours [10]. China dominated EV LIB manufacturing, while the United States and Europe experienced the most rapid market development [16]. Besides EVs, LIBs have seen widespread adoption in consumer electronics ranging from cellphones to power tools. Furthermore, LIBs also play a vital role in grid energy storage systems, as battery energy storage systems (BESSs) contribute to reliable energy supplies from storage grids and increase the economic viability of renewable energy sources. Currently, LIBs represent more than 90% of the global grid battery storage market [17].

The widespread use of LIBs and their high energy density introduces safety risks associated with thermal runaway (TR), which can result in fires, explosions, and hazardous emissions [18]. Hence, it requires significant effort to study TR carefully to understand its mechanisms and potential impacts and to develop strategies to avoid TR (the underlying mechanisms of TR will be discussed later in Chapter 2).

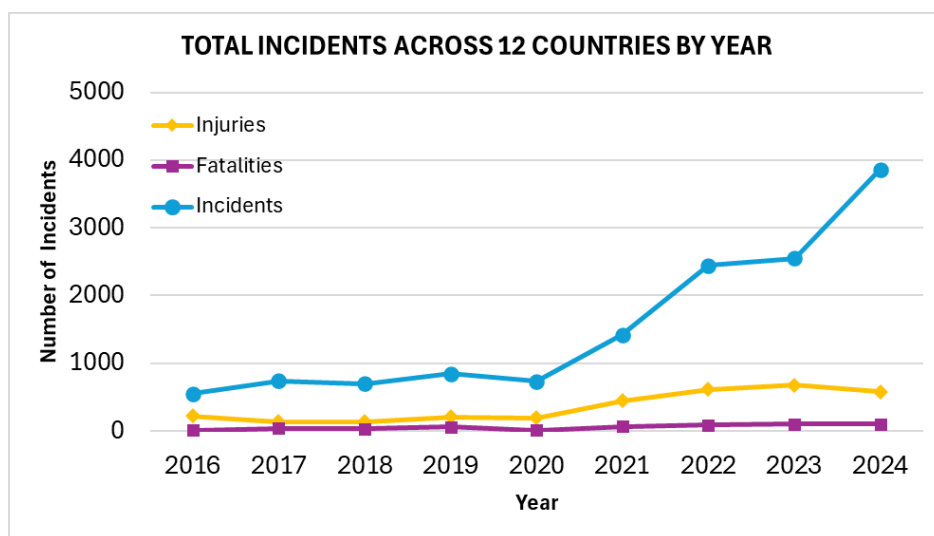
1.2 Increasing LIB Incidents

1.2.1 Global Rise in Battery Incidents

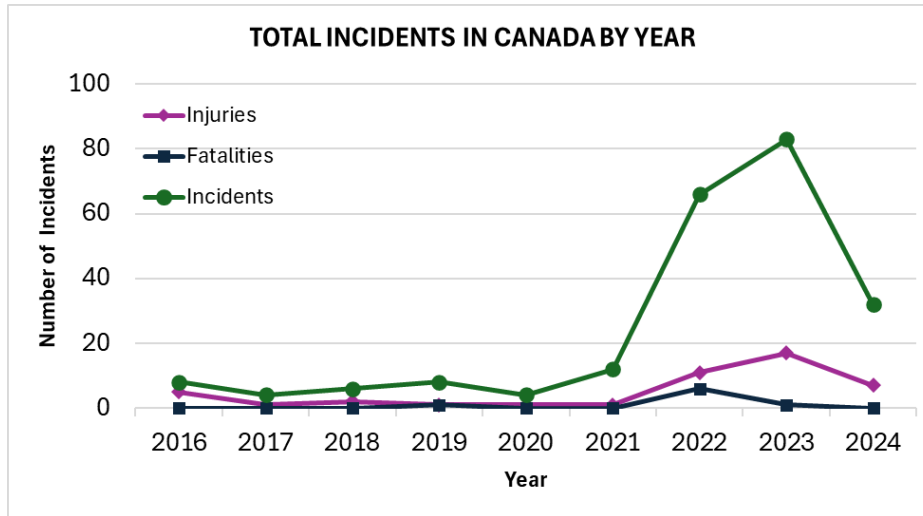
Concurrently with the expansion of the battery industry, there has also been an increase in safety incidents, prompting heightened attention from both consumers and manufacturers [19], [20], [21].

Figure 2 (a) illustrates the rising number of LIB safety incidents reported across 12 countries including Canada, China, Germany, India, Japan, the Netherlands, Norway, Singapore, South Korea, Sweden, the United States, and the United Kingdom, between 2016 and 2024. Similarly, a clear upward trend in the incidents over time is also observed in Canada, as shown in **Figure 2 (b)**. While TR is a mechanistic phenomenon at the cell-level, real-world battery incidents often represent system-level outcomes where TR initiation, propagation, and environmental conditions jointly determine the severity of fires, explosions, and hazardous emissions.

(a)



(b)



(c)

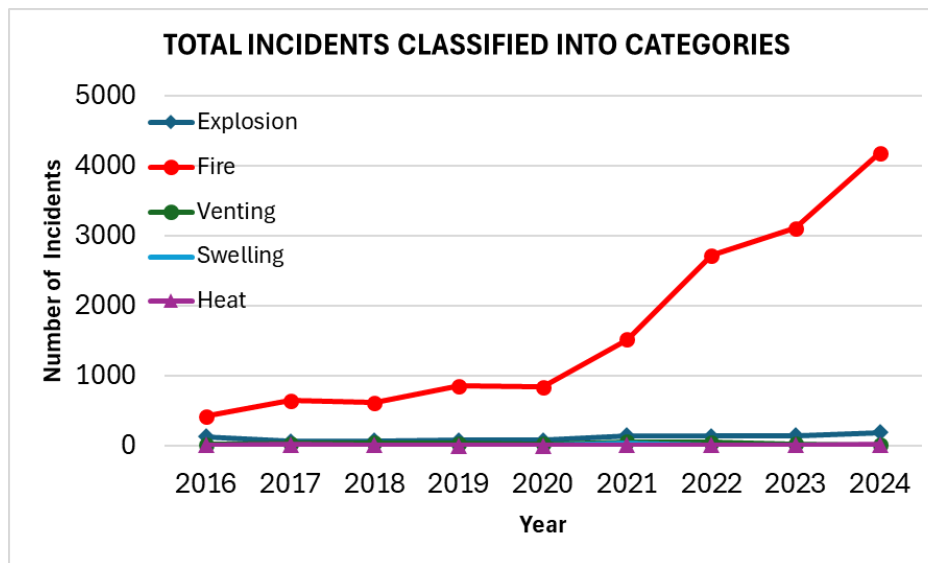


Figure 2: (a) Increase in incidents related to LIBs, e.g., injuries, fatalities, and incidents, in 12 countries between 2016 and 2024, (b) increase in incidents related to LIBs, e.g., injuries, fatalities, and incidents, in Canada between 2016 and 2024, (c) LIB incidents from 12 countries between 2016 and 2024 are classified based on battery status, e.g., explosion, fire, venting and heat. Recreated originally from [22]

(a)

1.2.2 Health and Environmental Hazards

Safety incidents involving EV batteries (e.g., LIBs) typically result in fires as shown in **Figure 2 (c)**, which can cause catastrophic passenger injuries and substantial reputational damage to battery manufacturers, ultimately hindering the wider adoption of emerging technologies. Moreover, incidents involving explosions, venting, and fires, along with the release of toxic emissions present significant hazards to human health and environmental safety [23], which are disastrous for the surrounding environment and affected individuals [22]. For example, HF (hydrofluoric acid) is one of the dangerous emission components that can cause eye irritation, skin burns, and respiratory diseases under prolonged exposure [15].

1.2.3 Notable Incidents in North America

Recent years have seen a few significant LIB incidents in North America. The City of Toronto recorded a 162% increase in LIB fires between 2022 and 2024 [24]. The City of Vancouver reported LIB fires as one of the leading contributors to urban fire incidents [25]. In September 2024, a fire involving LIBs on a ship in Montréal port released large volumes of HF gas and particulate matter (PM) into the atmosphere, severely polluting the environment and jeopardizing the health and safety of both firefighters and surrounding communities [26]. In the USA, reports from the first quarter of 2024 revealed a rising number of LIB fire incidents in New York City, where there were 267 LIB fires in 2023, leading to 150 injuries and 18 deaths [27].

As seen in **Figure 2 (c)**, fires are the most common outcome associated with LIB failure. Firefighters reported that extinguishing an EV fire caused by LIBs can require up to 3 h and 40 times more water compared to extinguishing a fire produced from an internal combustion engine that could be extinguished in only about 20 min [28], [29]. This presents significant challenges for firefighting, necessitating specialized equipment and training. However, a nationwide survey conducted in 2022 involving over 1000 USA first responders revealed that more than 40% of them received no safety training related to EV fires [30].

On the other hand, the hazards associated with LIB fires and their impact on human health are still unclear [31]. For example, to improve the understanding of the required decontamination procedures to ensure the safety of personal protective equipment (PPE), the Fire Protection

Research Foundation (FPRF) of the US National Fire Protection Association is currently conducting studies on LIB fires and the associated health risks on firefighter exposure [32].

1.3 Accelerated Testing of LIBs: Nail Penetration Tests

Due to hazards associated with TR, regulatory bodies increasingly require manufacturers to perform comprehensive safety testing of LIBs before commercialization [33], [34]. However, real-world TR events are complex and challenging to replicate due to system scale and associated risks [35]. For instance, the Federal Aviation Administration (FAA) has reported an average of about 1.4 fires per week caused by the LIBs transported through aircraft cabins in the year 2025 [36]. In another instance, a damaged e-bike battery pack caught a building on fire [37]. Replicating such real-life scenarios can be challenging because failure events vary. Manufacturers, therefore, develop accelerated testing protocols by raising the stress factor levels on the LIBs to hasten degradation levels [38].

In real-world applications, LIBs may be exposed to thermal, electrical, and mechanical damage [39]. Failure testing protocols must, therefore, replicate these scenarios. On the one hand, NP tests are a standard mechanical abuse test, simulating failures like those in vehicle crashes where sharp objects may penetrate the cell [40],[41],[42], [43]. A conductive nail in NP tests can create contact between the electrodes forming a conductive path that induces a short circuit [44], [45].

NP tests have become an important lab test in battery safety research, and the results are influenced by factors such as battery types and test conditions. Abaza et al. [46], for example, found that using conductive nails in NP tests causes greater temperature spikes than non-conductive ones. The emission profiles across NP tests can also differ when compared to one another. A study comparing various TR initiation methods found different quantities and concentrations of emitted gases even for the same cell chemistry [41].

1.4 Research Objectives

The objective of this thesis is to improve the understanding of nail penetration (NP)-induced thermal runaway (TR) in lithium-ion batteries (LIBs) through experimental investigation of both failure behaviour and particulate emissions. Although NP testing is widely employed to evaluate battery safety under mechanical abuse, uncertainties remain regarding the influence of operating

conditions on TR progression and the characteristics of particulate matter (PM) generated during failure events.

To address these knowledge gaps, commercially available LG-HG2 (INR18650HG2) cylindrical LIB cells were subjected to NP under varying states-of-charge (SOC) and low-temperature conditions representative of cold-weather operation. The resulting TR behaviour was evaluated through temperature measurements and visual observations to assess ignition characteristics, thermal response, combustion behaviour, and overall event severity.

A second objective was to compare the macroscopic TR behaviour of commercially available LIBs with different chemistries, capacities, and form factors. Visual observations obtained from NP tests were used to examine differences in ignition behaviour, venting characteristics, and combustion response, providing a broader understanding of how battery design influences failure behaviour under mechanical abuse.

The final objective was to characterize the particulate matter (PM) generated during NP-induced TR. Previous studies have reported the presence of carbonaceous residues, metallic particles, and fragmented electrode materials; however, the relationships between particle morphology, size distribution, composition, and their spatial distribution within the failed cell remain insufficiently understood. Therefore, particle size distribution (PSD) analysis, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD) were employed to characterize the morphology, elemental composition, and crystalline phases of the collected ejecta, together with the spatial distribution of decomposition products within the failed cell.

The findings of this work contribute to the understanding of NP-induced TR behaviour and particulate emissions from LIBs, supporting the development of improved battery safety assessment methodologies and providing insights into the mechanisms governing particulate formation during battery failure.

1.5 Thesis Outline

This thesis consists of seven chapters. Chapter 1 introduces the motivation for this research, outlines the safety challenges associated with LIBs, presents the research objectives, and provides

an overview of the thesis. Chapter 2 presents the background and literature review on LIB TR, NP testing methodologies, factors influencing TR behaviour, temperature measurements, and particulate characterization. Chapter 3 describes the experimental apparatus, test procedures, and the LG-HG2 cells investigated in this study. Chapter 4 presents and discusses the experimental results on NP-induced TR under varying SOC and low-temperature conditions. Chapter 5 compares the TR behaviour of commercially available LIBs with different chemistries and form factors. Chapter 6 investigates the particulate emissions generated during NP-induced TR using PSD analysis, SEM, EDX, and XRD. Finally, Chapter 7 summarizes the main findings of this work and provides recommendations for future research.

Chapter 2 Background

2.1 Thermal Runaway in LIBs: Causes, Consequences, and Test Methodologies

2.1.1 What is Thermal Runaway?

Safety incidents involving LIBs typically occur when the batteries enter thermal runaway (TR), which is a rapid uncontrollable heat-generating process driven by exothermic reactions. LIB modules are designed to operate within a specific temperature range and are typically equipped with battery management systems (BMS) to regulate heat dissipation through convection and ventilation. The optimal operating range of LIBs is typically between 15 and 35 °C and the recommended charging window is between 10 and 40 °C [47], [48]. However, when the internal or external heat generation surpasses the dissipation capacity, the BMS loses its ability to regulate the temperature rise.

The exothermic heat generation ignites the flammable electrolytes and results in high-speed fire ejecta through the cell vent. Gupta et al. [49] classify the propagation of this fiery ejecta into three ignition modes. The ejecta can take the form of a spark shower, localized fragments, or shell ejection. The spark shower depends on particle density, while the latter two modes are based on internal cell particles released during high-speed venting. As LIB cells are closely packed, TR can easily propagate onto the neighboring cells initiating a destructive failure.

2.1.2 Initiation Mechanisms and Reactions

The root cause of TR is short-circuiting that results from direct contact between the battery electrodes. This contact can be internal, formed because of separator damage, or when a conductive material penetrates through the electrode layers. The resulting localized high current density causes a rapid temperature rise, initiating a series of exothermic chain reactions within the cell that further elevate the temperature to exacerbate the condition [50].

One of the first processes is the vaporization of the electrolytic solvents, elevating the internal pressure. In pouch cells, this causes visible swelling, while in cylindrical or prismatic cells, the pressure is relieved through venting. The vented gases consist of flammable organic solvent vapors, which are prone to ignition either during or after venting due to their low flash point.

Concurrently, the solid electrolyte interphase (SEI) layer decomposes, which initiates further reactions between the anode and the electrolyte. At elevated temperatures, electrolyte breakdown results in the formation of hydrocarbons and HF. Additional gases such as C₂H₄ (ethylene), C₂H₆ (ethane) and C₃H₆ (propylene) form as the solvents react with the lithium metal of the cathode [51].

Understanding the solvent decomposition mechanism is critical to understanding TR. **Table 1** presents some of the dominant decomposition reactions of ethyl methyl carbonate (EMC), dimethyl carbonate (DMC), diethyl carbonate (DEC), and ethylene carbonate (EC), obtained from pyrolysis experiments.

Sun et al. [52] reported that DMC undergoes four dominant unimolecular decomposition pathways between 500 and 2300 K, as shown in **Table 1**. These include the formation of dimethyl ether (CH₃OCH₃) and carbon dioxide (CO₂) formed via R1. Bimolecular pathways such as R3 and R4 become increasingly favorable at higher pressures. Similarly, DEC is transformed into diethyl ether (C₂H₅OH), ethylene (C₂H₄), and CO₂ at temperatures between 700 K and 1200 K. Other reaction pathways that are not included in **Table 1** are possible at higher temperatures.

For EC, Kanayama et al. [53] identified R5 as the dominant pathway (300–3000 K), forming acetaldehyde (CH₃CHO) and CO₂, likely due to its lower activation energy. Takahashi et al. [54] studied EMC and found that it forms methoxy formic acid (MFA, COC*OOH) and C₂H₄ around 850 K, with MFA further decomposing to methanol (CH₃OH) and CO₂ at the same temperature. At 1050 K, secondary decomposition products such as carbon monoxide (CO) and CO₂ were also observed.

Table 1: Decomposition reactions of different electrolytic solvents

Solvent	Reactions #	Reaction	Type
Dimethyl Carbonate (DMC) [52]	R1	$\text{DMC} \rightarrow \text{CH}_3\text{OCH}_3 + \text{CO}_2$	Unimolecular
	R2	$\text{DMC} \rightarrow \text{CH}_3 + \text{CH}_3\text{OC}(=\text{O})\text{O}$	Unimolecular
	R3	$\text{DMC} + \text{H} \rightarrow \text{H}_2 + \text{CH}_3\text{OC}(=\text{O})\text{OCH}_3$	Bimolecular
	R4	$\text{DMC} + \text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OC}(=\text{O})\text{OCH}_2$	Bimolecular

Ethylene Carbonate (EC) [53]	R5	$EC \rightarrow CH_3CHO + CO_2$	Unimolecular
	R6	$EC \rightarrow C_2H_4O + CO_2$	Unimolecular
	R7	$EC \rightarrow C_2H_3OH + CO_2$	Unimolecular
Ethyl-methyl Carbonate (EMC) [54]	R8	$EMC \rightarrow C_2H_4 + COC^*OOH$	Unimolecular
	R9	$COC^*OOH \rightarrow CH_3OH + CO_2$	Unimolecular
Diethyl Carbonate (DEC) [55]	R10	$DEC \rightarrow C_2H_5OC(=O)OH + C_2H_4$	Unimolecular
	R11	$C_2H_5OC(=O)OH \rightarrow C_2H_5OH + CO_2$	Unimolecular

In addition to the electrolyte, the cathode material begin decomposing at temperatures between 200 and 600 °C [56], releasing oxygen due to its lithium oxide content. This oxygen acts as an oxidizer, sustaining combustion [51]. Each cathode chemistry influences TR differently, so individual decomposition pathways are not detailed here. For example, comparative experiments reveal that NMC-based cells emit higher volumes of hazardous gases and propagate TR more readily than LFP cells, indicating chemistry-dependent risk profiles [57].

The severity of TR depends on both the total energy stored in the battery and the magnitude of current through short circuits. Electrolyte and cathode decomposition supply the fuel and oxidizer required to sustain a fire, while the heat generated from the short circuit during TR completes the fire triangle. A self-sustaining fire alongside toxic emissions makes LIB fires incredibly difficult to extinguish [57], [58].

2.1.3 Thermal Runaway Triggers

TR can be induced by many factors, including internal manufacturing defects as well as external triggers such as overheating, overcharging or mechanical damage [59], [60], [61]. Generally, overheating can cause the separator to shrink or melt, increasing the risk of internal short circuits [62]. Meanwhile, overcharging, which occurs when a battery is charged beyond its cutoff voltage or 100% SOC, leads to lithium plating on the anode. Over time, these lithium deposits may form dendrites that could pierce the separator and initiate internal shorts [63],[64]. Overcharging can

also increase the internal cell temperatures, accelerating the decomposition reactions described earlier, and heightening TR risk.

Mechanical damage can be caused by external events such as vehicle collisions or internal processes like vibration-induced micro-cracks in the separator [65]. Manufacturing impurities and lithium dendrite growth during regular operation are also known contributors to separator damage [59], [66]. In EV packs, where many cells are interconnected, the failure of even a single cell can lead to TR propagation [67],[68] . The intense heat during a TR, sometimes as high as 700 °C, can easily spread to neighboring cells and modules [69].

2.2 Nail Penetration Test Methodologies

Nail penetration (NP) tests are usually performed in an NP test rig housed in a fire-proof and explosion-proof chamber. First, LIB cells to be tested are placed on an insulation plate in the test rig, as illustrated in **Figure 3**, where a cylindrical cell is used as an example. The cells need to be securely positioned between a dedicated fixture so that they don't move during NP tests. The enclosed test chamber is generally capable of withstanding LIB fires to a certain degree. A well-designed chamber can maintain a controlled atmosphere (usually inert). The emission from TR tests can be extracted using gas sampling lines in the chamber or from the exhaust. As the test parameters can significantly influence the test outcomes, well-defined methodologies are essential to ensure both reproducibility and the collection of meaningful data from NP tests. In this section, NP studies reported in the last decade are reviewed with a specific focus on the characterization of the generated emissions.

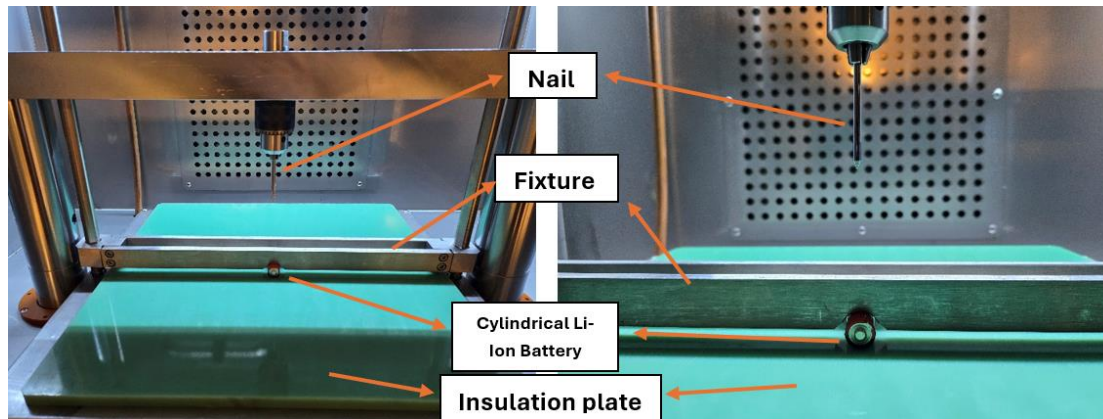


Figure 3: Photos from two angles of a nail penetration (NP) test example rig. A cylindrical Lithium-ion battery is used as an example

One of the earlier studies on LIB TR emission characterization was conducted by Nedjalkov et al. [44]. They tested NMC pouch cells within a plastic barrel, and the exhaust followed a series of filters and analytical instruments installed downstream for characterization. A common configuration as such has been employed in several studies where the cells are enclosed in a chamber, and the emissions are directed into an analyzer. Koch. et al. [42], for instance, tested LIB modules in an aluminum housing. The modules have similar cathode chemistry but different capacities.

Test procedures of NP experiments are designed to obtain varying test objectives, which are seen throughout the works reviewed. For example, although both Koch et al. [42] and Nedjalkov et al. [44] examined NMC pouch cells, their objectives differed and hence, the test procedures were different. Nedjalkov et al. focused on emission characterization, and prevention methods of toxic gases using filters, whereas Koch et al. aimed to assess the effectiveness of sensors in TR detection. As a result, their procedures also varied. Nedjalkov et al. slightly overcharged (above 100% SOC) the cells to ensure TR, while Koch et al. preconditioned the cells to 60 °C and full SOC before initiating NP.

Preconditioning the cells prior to testing is an important step in NP experiments, as the cell condition could lead to different NP results. Diaz et al. [70] performed a comprehensive analysis of LIB NP by comparing emissions across multiple cell chemistries and formats, including LCO, LFP, and NMC cells in both cylindrical and pouch configurations. A nitrogen (N₂)-filled chamber

was used with gas analyzers positioned downstream. Unlike earlier studies, they did not overcharge or preheat the cells, which resulted in several 50% SOC cells failing to undergo TR.

Special cell fixture designs may be required to obtain a more precise emission characterization. For example, Essl et al. [41] adopted a more advanced chamber design to test pouch and prismatic NMC cells. The test configuration was similar to that of Diaz et al. [70] and Nedjalkov et al. [44], but great importance was placed on the design of the cell fixture. The custom-designed chamber consisted of two stainless steel holders for the cell, separated by mica sheets to prevent any thermal conduction to the test rig. It was pressure-sealed and filled with N₂. Gas sensors were placed inside the chamber in addition to other analytical instruments positioned downstream of the chamber. Compared to the plastic barrel setup used by Nedjalkov et al. [44], where no carrier gas was reportedly used, the controlled chamber environment used by Essl et al. [41] and Diaz et al. [70] allowed a more precise emission characterization.

Different experimental approaches have been developed to study emissions during NP-induced TR. Hoelle et al. [71], for instance, used an autoclave calorimeter to test NCA and NMC prismatic cells under tightly controlled conditions. The cells were wrapped on all sides using copper blocks to restrict expansion and isolate heat transfer, allowing a detailed assessment of mass loss and heat generation during TR. Although the study tested 50 cells in total, only the emissions from one out of the 50 samples were analyzed, limiting the generalizability of the observations.

Environmental and testing conditions have been shown to significantly influence both the onset and severity of TR, including the emission characteristics. Doose et al. performed NP tests in sealed chambers equipped with humidity-controlled bubblers and voltage-dependent nail control, and the nail movement was automatically halted upon voltage drop, thereby improving the reproducibility of short-circuit initiation [43]. This configuration was utilized in another study by Diekmann et al. to assess the impact of nail geometry on TR behaviour, with some tests following the SAE J2464 protocols to ensure procedural consistency [72].

While most emission studies of NP have relied on closed systems to minimize ambient contamination and ensure accurate sampling, open-air configurations have also been explored in some studies. In one such study, Willstrand et al. [45] tested NMC prismatic cells in both open and closed chambers. The closed chamber was a concealed pressure vessel with inert N₂, and the emissions from TR were left to accumulate within the chamber making it possible to assess the

generated gas volume. In the open configuration, the test rig was placed under a fume hood, with insulation panels directing the gaseous emissions upward for sampling. Although the design introduces a greater operational risk, it offers a realistic scenario of TR events. Similar open-air testing was conducted in another study involving modular LIBs, where the goal was the characterization of PM and emissions [57]. For this purpose, a comprehensive array of particle analyzers and emission samplers was integrated into the test rig. In both cases, however, emission sampling becomes more challenging due to diffusion and varying ignition behaviour of the cells under TR. More recent comparative studies by Howard et al. employed both open-configuration NP testing and sealed pressure vessel configurations to test NMC and LFP chemistries. In the open configuration, the test rig was exposed to the atmosphere, and the gas samples were collected through a sampling vent. In the closed configuration, a pressure vessel was purged multiple times with inert gases (argon or nitrogen) prior to NP testing. The gas sampling was conducted only after temperatures returned to ambient inside the pressure vessel. The instruments used in sampling were calibrated for a few target gases [73], [74].

Reeve et al. conducted NP tests inside a reinforced pressure vessel originally developed for closed-system failure analysis [75]. Cells were first diagnosed through cathode verification using XRF and instrumented with surface thermocouples before being mounted in a baffle-protected holder within the vessel. The internal atmosphere was repeatedly purged with inert gas to stabilize oxygen concentrations prior to testing. TR was initiated by driving a hardened stainless-steel nail of 3 mm diameter at 10 mm/s. To ensure a homogenous environment, a fan was used to continuously mix the gases before being sampled into Tedlar bags [75].

A more advanced methodology was implemented by Walker et al. in a large-format fractional thermal runaway calorimeter (L-FTRC) designed to quantify total and fractional heat output from large-format prismatic cells while maintaining flight-representative mechanical constraints as the cells tested were designed for satellite use. The cells were penetrated using a tungsten nail and the emissions were directed into an argon purged collection system [76].

In summary, methodological differences have been observed across recent NP studies. To ensure reliable and reproducible results, several factors must be carefully controlled. These include cell parameters such as capacity, SOC, and cathode chemistry, which significantly influence TR behaviour, as well as test conditions and rig design, which determine the accuracy of

measurements and the likelihood of ignition. Closed chambers enable precise quantification of vent-gas composition and mass loss, while open-air configurations offer clearer visualization of TR dynamics but are highly susceptible to ignition. Maintaining consistency in both the relevant cell parameters and the experimental conditions is essential for generating comparable NP data.

2.3 Observations during Nail Penetration-Triggered Thermal Runaway

The outcomes of LIB NP-experiments vary significantly as they are largely influenced by cell parameters and are highly susceptible to test conditions. Generally, a drop in cell voltage is observed immediately after NP, followed by a rise in cell temperature [43]. This is typically followed by the venting of ejecta, which results from internal gas generation and the subsequent pressure increase [71]. In some cases, venting can lead to cell rupture and fire [44]. At the cell-level, differences in NP outcomes are more apparent. For example, Reeve et al. [75] reported that cylindrical cells failed at the vent cap or positive terminal during other abuse tests, but not during NP. This is likely due to the alternative venting path created during the nail insertion.

The comparative study by Essl et al. [41] on pouch and prismatic cells found that hard-case prismatic cells could withstand a higher internal pressure (i.e., 855 kPa) before venting, compared to pouch cells (411 kPa). As the tests were conducted in an inert atmosphere, no fires were reported. In contrast, Diaz et al. [70] observed that some pouch cells underwent severe TR under inert conditions, leading to the melting of the cell casing, while others only experienced swelling. SOC played a significant role in the NP results: for cells at 50% SOC, only visible swelling was observed, while cells at higher SOC had TR triggered by NP.

Diekmann et al. [72] reported that vent gases ignited under an oxygen-rich atmosphere, while under inert nitrogen, the ejecta glowed but did not ignite. Meanwhile, Willstrand et al. [45] found inconsistent ignition results when testing cells in open configuration, some ignited even at low SOC (25%), while others did not. The cause of this disparity is unclear, but it had a direct effect on gas emissions, particularly CO₂ and CO concentrations. Cells that ignited released greater amounts of CO₂.

Later studies suggest that NP test outcomes are influenced by the cathode chemistry [73], [74] as is evident from the NP tests performed on LFP and NMC pouch cells. The LFP cells did not show

any signs of TR, and only a slight swelling was observed in the NMCs. In contrast, another recent work discovered that fully charged pouch cells behaved differently under inert conditions despite identical cathode chemistries [77]. The cell with lower capacity and volume was found to undergo a more severe TR, marking a disparity with previous findings.

These studies collectively show that NP-induced TR outcomes are highly inconsistent across the literature due to variations in cell parameters, cathode chemistry, and the test environment. As a result, findings often appear contradictory: some studies report no ignition under inert conditions, while others observe severe TR; some cells rupture dramatically, whereas others only swell, and even cells with identical chemistries can behave differently depending on capacity and construction.

The key message of this section is that NP outcomes cannot be generalized across studies. Instead, they depend strongly on the specific interplay between the cell properties and the experimental setup used. Understanding these dependencies is essential before drawing conclusions or comparing results across NP investigations.

2.4 Influence of Cell Parameters on NP Results

2.4.1 Cell Capacity

Cell capacity is a key parameter in determining the TR hazard during NP tests, because of the total stored energy within the cell that can intensify the heat generation during an induced short-circuit.

Results from Nedjalkov et al. [44], Essl et al. [41] and Premnath et al. [57] can be compared to demonstrate the effect of capacity on NMC pouch LIB NP test results using varying methodologies. Nedjalkov et al. [44] conducted tests on 40 Ah cells in a sealed chamber with comprehensive analytical tools. Their results revealed a wide range of emission species, including multiple hydrocarbons, solvent vapors, and alcohol compounds. However, Essl et al. [41] and Premnath et al. [57] used slightly higher capacity cells (58–65 Ah/cell), and detected various other hydrocarbons in the emissions from NP tests. The findings from all three studies, however, do not completely overlap, which is likely because they were influenced by their test setups and environments. Premnath et al. [57] performed NP on modular LIBs in an open setup, but Essl et al. [41] and Nedjalkov et al. [44] conducted cell-level experiments in enclosed chambers. In

addition, an inert atmosphere was maintained in the chamber in [41], while no such measures were taken in [44].

The results for NMC prismatic cells can be compared in Essl et al. [41], Hoelle et al. [71], and Willstrand et al. [45]. Hoelle et al. explored a broad range of cell capacities (i.e., 8–145 Ah), while Essl et al. and Willstrand et al. tested cells at 60 Ah and 157 Ah, respectively. According to these studies, the total gas generation per unit capacity ranged from 1.77 to 2.06 L/Ah, suggesting a correlation between cell capacity and gas evolution. The observed variation in gas volume appears to correlate with differences in stored energy, indicating the influence of capacity on TR outcomes.

2.4.2 Test Environment

The test environment plays a crucial role in shaping TR behaviour during NP experiments. Open test rigs could not control the test environment, and only a few papers reported their studies conducted in open test rigs in room air. Willstrand et al. [45] observed that cells tested in open configurations had slightly lower TR onset temperatures compared to those in closed and inert chambers. The temperatures ranged between 130 °C and 210 °C depending on the SOC. Notably, fires were initiated at SOCs as low as 25% in the open tests, suggesting increased flammability under these conditions. Similarly, Premnath et al. [57] reported fires in most of their NP test cases of battery modules in an open rig. The fires occurred due to the readily access of air in the open rig setup, and the high energy content in the battery modules also contributed significantly to the larger fires and greater quantities of combustible gases emitted. However, an LFP module that underwent NP tests was reported not catch fire [57]. The fact that LFP cells are difficult to ignite was also confirmed in Howard et al. [73], where LFP cells of different capacities were found not to undergo failure during NP tests, let alone a TR.

Most closed-chamber experiments were conducted in inert atmospheres such as nitrogen or argon, which may suppress ignition during NP tests. However, Diekmann et al. [72] noted that the use of oxygen-filled atmosphere can create overpressure conditions within the chamber, which may influence the TR onset. In their comparative study on LCO pouch cells using compressed air and N₂ in a closed chamber, they observed ignition events only in NP tests in air-filled chambers, along with a notable spike in short-term pressure. The pressure was approximately 1.48 bar during the deflagration in air, while it was only half as much in a N₂-filled chamber. Interestingly, the maximum TR temperatures remained similar across tests conducted in both atmospheres. This may

suggest that the observed differences in TR temperatures for tests conducted in open and closed chambers in [45] may be due to the confinement conditions rather than to the gas composition alone.

Gas production rates differ in tests conducted in different environments, e.g., air, inert, or humid N₂, but different trends are reported in the literature. For example, Diaz et al. [70] found that inside the enclosed test chamber, using air as a carrier gas for the TR emissions resulted in measuring greater emission volumes than when N₂ was used as the carrier, indicating that the oxidative environment may enhance gas generation. In contrast, a different trend was reported in [74] where an average net gas volume of 10.7 L was emitted in a N₂ atmosphere, and only 8.9 L was emitted in the presence of air. In this study, they used a pressure vessel for NP. Another study uniquely incorporated humidity control into its chamber design using a bubbler system. Their results showed that increased humidity within a N₂ environment promoted condensation of vapour-phase products on chamber surfaces, reducing the concentration of measurable gaseous species [43].

In summary, these studies demonstrate that while inert environments may not significantly alter TR temperature thresholds unless coupled with pressure effects, they do influence the total gas generation and combustion behaviour. Therefore, variables such as confinement, oxidizing atmosphere, and humidity should be carefully considered when designing NP test environments. Results obtained in different gas environments should also be compared with special care.

2.4.3 Nail Characteristics

The influence of nail characteristics in NP tests can be analyzed from two perspectives. The first are the operational parameters, including the penetration speed and depth of insertion, while the second involves the geometry and material of the nail, such as diameter, tip angle, and conductivity.

Nail penetration speed can impact the reproducibility of NP results. Diekmann et al. [72] examined the influence of penetration speed (e.g., 1 mm/s, 5 mm/s, 10 mm/s, 40 mm/s, and 80 mm/s) and found that using a penetration speed of 1 mm/s, much lower than the 80 mm/s suggested in SAE standards, could significantly lower standard deviations in temperature and voltage profiles. This slow penetration rate was found to be able to allow for more stable and consistent triggering of TR [72]. This low penetration speed (i.e., 1 mm/s), was later adopted by other researchers, such as Doose et al. [43].

The penetration speed also appeared to play a role in the composition of solvent vapor in the emissions from NP tests, which was found to be impacted by the residence time. Faster penetration rates (e.g., 80 mm/s) may limit the residence time required for intermediate reactions, leading to a higher fraction of unreacted solvent vapors in the final emission mixture. This may also explain the reason why low penetration speeds produce more reproducible results, as the generated gases get almost equal residence time before venting [72].

In addition, one might expect that increasing the diameter of a conductive nail would allow higher short-circuit currents, potentially intensifying the TR event. However, based on a NP study on LCO cells using various nail diameters (i.e., 2–5 mm) and tip angles (i.e., 20–40°) [43], it was found that nail geometry did not significantly affect whether TR occurred or how severe it was. The authors attributed the outcomes to the dominant influence of the low penetration speed (i.e., 1 mm/s), which may limit short-circuit current regardless of nail size. More studies are needed to confirm this.

In terms of nail material, Diekmann et al. [72] noted that using conductive nails as opposed to non-conductive ones enhanced reproducibility. Conductive nails directly contact the electrodes during penetration, ensuring a short-circuit event, whereas non-conductive nails may not directly connect the internal layers, delaying or weakening the trigger.

Based on these findings, recent studies focusing on characterizing the emissions from NP tests tend to fix nail characteristics (especially penetration speed) to ensure consistent TR triggering in the tests [73], [74]. However, the influence of nail material and shape under different conditions, such as faster penetration speeds or varying cell chemistries remains underexplored

Overall, these findings suggest that while slow penetration speed and conductive nails are preferred in NP tests to enhance the reproducibility, the role of geometry in influencing TR is not yet conclusive. Further studies are needed to determine whether these observations hold true across cell formats, SOC levels, and more sophisticated test setups.

2.4.4 State-of-Charge (SOC)

The state-of-charge (SOC) plays a critical role in determining the likelihood and TR severity during NP. Most experimental studies were conducted at 100% SOC, as this condition is more

likely to trigger TR and allow researchers to assess the worst-case scenarios [42], [44], [73]. Conducting NP tests on fully charged batteries seems to become a standard practice in the literature.

However, there are a few studies that explored the SOC effects on NP results, such as [70] and [45]. Diaz et al. [70] performed NP on LCO pouch cells in an open environment, and they found that only cells with 100% SOC experienced TR during NP tests, while the cells at 50% SOC exhibited only swelling and gas release but did not enter runaway. A more recent study also observed that only NMC pouch cells at full charge experienced TR conditions during NP tests regardless of the test environments [74]. On the other hand, Willstrand et al. [45] used a closed chamber setup and tested high-capacity NMC prismatic cells. They observed TR for cells at both 25% and 100% SOC, while the peak temperature during TR was significantly higher for cells at 100% SOC. This suggests that while TR can still occur at lower charge levels in large-format cells (e.g., prismatic), the severity of the event increases with SOC.

Overall, these findings highlight that batteries with different SOC levels can demonstrate different TR behaviours, but the impact of SOC is also intertwined with cell format, capacity, and the test environment. Future studies that decouple these variables could provide more generalized insights into the SOC-TR relationship.

2.5 Temperature Measurement in Nail Penetration Tests

Temperature is a key indicator in TR studies, as it informs the design requirements for the thermal protection systems capable of withstanding high heat fluxes from cell surfaces and vent emissions. Temperature profiles during NP tests are usually measured using thermocouples, but different placement strategies exist based on the test setup and objectives of the study. For example, Koch et al. [42] positioned a K-type thermocouple on the module surface near the NP site, likely aiming to capture an average surface temperature, while Essl et al. [41] placed thermocouples at multiple points, including the cell surface and tabs, sandwiched between insulation sheets. This multi-thermocouple setup enabled them to isolate the peak cell temperature from the vent gas temperature, an advantage in detailed thermal characterization.

Closed-chamber setups impose constraints on thermocouple placement due to space limitations, whereas open setups provide greater flexibility for thermocouple placement. For example, Premnath et al. [57] installed 15 thermocouples around the module and an additional six inside the

exhaust duct, including one for measuring ambient temperature. Willstrand et al. [45] opted for a minimal configuration with four thermocouples: three on the cell surfaces and one on the safety vent. Others integrate thermocouples into the nail itself to monitor internal cell temperature during penetration, helping them highlight a correlation between nail depth and TR severity [72].

While most studies rely on type K thermocouples for their affordability and wide temperature range, type N thermocouples were also used as in [73], [75], and [77] with an improved performance at high temperatures. However, type N thermocouples are usually at a higher price [78].

In summary, thermocouple quantity and placement are both critical. While embedding sensors inside the nail offers insight into pre-TR temperature rise, external placement near vents enables accurate tracking of emission heat profiles. Proper insulation and strategic positioning help minimize heat losses and avoid interference with the cell's failure behaviour.

2.5.1 Temperature Profiles of Different Battery Types and Configurations

Temperature peaks during NP tests vary significantly based on cell chemistry, form factor, SOC, and measurement strategy depending on whether TR occurs or not. Premnath et al. [57] reported that the thermocouple located beneath the NP site consistently recorded the highest temperatures during TR. This was confirmed across multiple tests, particularly for LFP modules. Their study also highlighted the stark contrast in peak temperatures between batteries of different chemistries: NMC modules were found to reach up to 900 °C, while LFP modules peaked at only 175 °C.

The trend that LFP batteries exhibit less severe results than NMC ones during NP tests was confirmed by multiple independent studies. Howard et al. [73] reported that during NP of LFP prismatic and pouch cells, no TR, fire, or visible failure indicators such as smoke were observed. Surface temperatures for these LFP cells remained low, ranging from 19 °C to 46 °C. On the other hand, they found that the NMC cells reached a maximum temperature ranging from 1010 °C to 1038 °C under NP-induced TR [74]. This suggests a strong thermal stability for LFP cells under NP conditions, especially when compared against chemistries such as NMC and LCO. Similarly, Essl et al. [41] reported a large temperature rise in NMC cells, with the surface temperatures reaching 782 °C for NMC pouch cells, and 777 °C for prismatic cells. However, Koch et al. [42] observed significantly lower temperatures (200–350 °C). This was because, the thermocouples in

[42] were placed inside the aluminum housing without making contact with the cell surface while in [41], they were in contact with the cell surface inside the confined-inert reactor.

Vent gas temperatures can be significantly different from the surface temperature of the battery cells. For example, the pouch NMC cell emitted gases at around 356 °C during NP tests, while the vent gas from a prismatic NMC cell could reach 1035 °C, although similar surface temperatures for both pouch and prismatic NMC cells were found [41]. This disparity is likely due to structural differences: pouch cells tend to rupture and release gases more diffusely due to swelling, whereas prismatic and cylindrical cells vent through a defined burst plate, enabling more focused and measurable gas streams.

For LCO pouch cells, different temperature profiles were reported. For example, Diaz et al. [70] estimated a maximum temperature exceeding 700 °C during TR based on visual evidence of a melted aluminum casing, while Diekmann et al. [72] recorded only about 500 °C based on the measurement using a high-accuracy, glass fiber tape-insulated thermocouple. This discrepancy reflects uneven temperature distributions during NP tests and emphasizes the need for standardized, robust temperature measurement protocols in NP studies. For example, cell surface temperatures and vent gas temperatures may vary depending on the cell form factor and therefore, must be accounted for when positioning temperature sensors.

2.5.2 Influence of Test Environment on Thermal Runaway Temperatures

The surrounding environment plays a critical role in determining the temperature profile of LIBs during NP tests, but this factor remains underexplored in many studies. Willstrand et al. [45] observed that ambient conditions significantly altered the maximum recorded temperatures. For NMC prismatic cells at 100% SOC, the ones tested in an open setup reached peak temperatures between 665 °C and 725 °C, while those tested inside a closed N₂-chamber exhibited much higher values, ranging from 838 °C to 857 °C. This suggests that heat dissipation is more constrained in a closed chamber, leading to higher localized temperatures. Although the cell chemistries differ, a comparable trend was observed in the study by Howard et al. [73], who used LFP cylindrical cells. In the inert gas environment (e.g., argon or nitrogen), cell temperatures ranged between 98 °C and 260 °C, while in air, the maximum surface temperature reached only 46 °C.

The composition of the test atmosphere has a pronounced effect. Diekmann et al. [72] reported that in a nitrogen-filled chamber, the battery only reached a maximum temperature of 47 °C,

compared to 122 °C in an air-filled chamber, an 88.7% increase. This finding underscores the suppressive influence of inert gases on combustion-driven temperature rise. Despite these insights, there remains a lack of systematic data on how environmental factors like ambient temperature or humidity influence the overall temperature profile during TR. It is plausible that increased humidity in the surroundings may reduce both surface and vent gas temperatures due to enhanced evaporative and convective cooling. But more studies are needed to confirm this.

2.6 Particle Characterization: Literature Review

Thermal runaway (TR) in lithium-ion batteries (LIBs) involves complex multiphase emissions, including gases, liquid condensates, and solid particulates. A substantial body of research has focused on characterizing solid particulate emissions generated during thermal abuse (TA) and mechanically induced failure conditions. Although most studies considered here involve 18650-format cells, the reported chemistries vary widely, including NMC (LiNiMnCoO_2), NCA (LiNiCoAlO_2), LFP (LiFePO_4), LTO ($\text{Li}_4\text{Ti}_5\text{O}_{12}$), and hybrid layered oxides such as $\text{Li}[\text{Ni}_x\text{Co}_y\text{Mn}_z]\text{O}_2$. This diversity in chemistry, coupled with methodological differences, leads to substantial variability in reported particle morphology, size distribution, and composition.

2.6.1 Real-time Aerosol Characterization Approaches

Claassen et al. investigated LCO 18650 cells using real-time aerosol monitoring techniques, including a cascade impactor and an Electrical Low-Pressure Impactor (ELPI+), enabling time-resolved measurement of particle number, size, and mass distributions over a range of 6 nm to 10 μm at different states of charge (SOC). Their results showed that increasing SOC led to higher particle generation, with ~ 100 nm particles dominating the distribution [79]. This study highlights the value of real-time diagnostics in capturing transient particle formation dynamics during TR, in contrast to post-mortem approaches that cannot resolve temporal evolution.

Zhang et al. further extended aerosol-based analysis to inhalable particulate emissions from NMC 18650 cells subjected to NP-assisted TA. Their results showed a strong submicron dominance, with most particles below 1 μm , emphasizing the respirable fraction of TR emissions. Sulfur-containing species were also detected, attributed to electrolyte additives or impurities [80].

However, the study relied on filter-based collection followed by aqueous detachment and ultrasonication, which may alter the native particle morphology and introduce bias in PSD interpretation.

2.6.2 Post-mortem Particulate Collection and Morphology Studies

Barone et al. examined aerosols emitted from NMC, LTO, and LFP cells subjected to TA in an accelerating rate calorimeter (ARC). Particles were collected on filters and analyzed using SEM-EDS. The study identified three primary particulate classes: nanoscale particles (30–100 nm), microspheres (0.1–3 μm), and larger electrode fragments (5–10 μm) [81]. Cathode-derived particles were typically spherical and contained Ni, Mn, and Co, while microspheres included metal-rich and mixed F/O/C compositions. However, the use of filter-based aerosol sampling limits direct comparison with bulk ejected powder studies due to preferential capture of fine particulates.

Ubaldi et al. conducted a systematic toxicity and elemental study of emissions from NCA, LFP, and LTO cells under controlled TA in a stainless-steel reactor. Solid emissions were captured on PTFE filters under both air and nitrogen atmospheres and analyzed using ICP-OES/AAS and ATR-FTIR. For NCA cells, dominant metals included Al, Co, Cu, Li, and Mn, while species such as Fe, Ni, and P were below detection limits, with P suggested to volatilize during TR. A key limitation is the absence of SEM/EDS-based morphological analysis, preventing correlation between chemical composition and particle structure [82].

In a complementary study, Ubaldi et al. also performed SEM-EDS analysis of filter-collected emissions from NCA 18650 cells. Particles exhibited largely spherical morphologies, with size-dependent compositional variation: smaller particles ($\sim 1\text{--}2\ \mu\text{m}$) were dominated by C, O, and F, while larger particles ($\sim 8\ \mu\text{m}$) contained Ni-rich phases with Al and Cu contributions. Atmospheric conditions also influenced morphology, with air environments producing smaller and more spherical particles compared to nitrogen [83]. However, the study did not include particle size distribution analysis or alternative chemistries such as NMC, limiting broader generalization.

Chen et al. investigated NMC 18650 cells using a dedicated ejected powder collection system under varying SOC and atmospheric conditions. Extensive multi-technique characterization

(SEM-EDS, XRF, ICP-OES, XRD, FTIR, GC-MS, and thermal analysis) revealed a highly heterogeneous powder consisting of carbonaceous species, metal oxides, silicon compounds, and polymeric residues. Carbon was the dominant constituent (~79 wt%), indicating strong contributions from electrolyte decomposition and binder degradation [84]. However, particle grinding prior to analysis likely altered the native size distribution, limiting direct PSD interpretation.

He et al. examined internal electrode degradation during TR by extracting anode and cathode materials post-heating of NMC cells. Their results showed extensive decomposition of cathode active material, with no intact NMC particles remaining on the cathode. Instead, LiF, Li₂CO₃, and transition metal oxides were detected, along with redistributed NMC fragments on carbonaceous surfaces [85]. However, this study focused on internal electrode surfaces rather than externally ejected particulates, limiting direct comparison with aerosol or ejecta-based studies.

Zhou et al. studied NMC811 cells subjected to combined NP and TA at high SOC. SEM and EDX mapping revealed heterogeneous distributions of C, O, Ni, Co, Mn, Cu, Al, F, and P across emitted particles, with carbon and oxygen dominating overall composition. XRD confirmed formation of metallic phases (Ni) and oxides (NiO, MnO, MnO₂) alongside electrolyte-derived LiF and Li₂CO₃ [86]. While this study captures realistic multi-stress failure conditions, quantitative PSD and spatially resolved EDX mapping across all particles were not provided, limiting statistical interpretation.

2.6.3 Particle Size Classification and Fractionation Studies

Garcia et al. investigated NMC811 cells using ARC-based TR followed by controlled decanting and sieving of emitted particulates into size fractions. SEM, ICP-OES, and TGA/DSC analyses were performed across these fractions. Particle sizes ranged broadly from <100 µm to >2 mm, with size-dependent compositional variation. While this study provides valuable size-resolved chemical insight, the relatively coarse fractionation limits resolution of fine particulate distributions, particularly in the submicron regime, and does not capture nanoscale emissions [87].

Grossetête et al. studied large-format prismatic NMC cells under TA. SEM-EDX study of individual particles revealed heterogeneous composition, with carbon-rich regions coexisting with

agglomerates containing Ni, Co, Mn, and O, attributed to NMC oxide fragments. Particle size distributions were obtained via laser analysis across broad bins (0–75 μm , 75–150 μm , 150–500 μm). However, EDX analysis was limited to individual points rather than statistically representative particle populations, preventing correlation between morphology, chemistry, and size distribution [88].

2.6.4 Methodological Trends and Recent Advances

Across the literature, two dominant methodological approaches emerge: real-time aerosol monitoring and post-mortem particulate characterization. Real-time techniques (e.g., ELPI+, impactors) provide temporal resolution of particle formation but limited chemical detail. In contrast, post-mortem approaches (filter collection, powder decanting, or electrode extraction) enable detailed chemical and morphological characterization but lose information on transient formation dynamics.

A further subset of studies incorporates mechanical–thermal coupling or complex abuse scenarios, revealing that combined stress conditions significantly influence particle morphology and composition but are rarely accompanied by quantitative PSD or statistically strong EDX mapping.

Chemical characterization is consistently performed using SEM-EDX, often complemented by XRD, ICP-OES/MS, FTIR, and XPS. However, many studies rely on qualitative interpretation of SEM images and localized EDX point analysis rather than full-field compositional mapping or particle-by-particle statistical analysis. A summary of the studies reviewed in this section can be found in **Table 2**.

Table 2: Summary of previous studies on thermal runaway particulate characterization

Study	Cell	Techniques	Main Findings	Key Limitation
Claassen et al. [79].	LCO 18650	ELPI+, impactor	~100 nm particles dominated emissions; higher SOC increased particle generation	No morphology or composition analysis
Ubaldi et al. [82]	NCA, LFP,	ICP-OES/AAS, ATR-FTIR	Detected Al, Co, Cu, Li, Mn in solid emissions	No SEM, EDX, or PSD

	LTO 18650			
Ubaldi et al. [83]	NCA 18650	SEM-EDX	Spherical particles; composition varied with particle size	No PSD; focused on NCA
He et al. [85]	NMC 18650	SEM-EDS, XRD, XPS, FTIR	Cathode decomposition produced oxides and fluorides	Internal electrodes only; no emitted particles
Chen et al. [84]	NMC 18650	SEM-EDS, XRD, ICP-OES, FTIR	Carbonaceous powder with metal oxides and silicon compounds; PSD reported	Grinding altered morphology and PSD
Zhou et al. [86]	NMC 18650	SEM-EDX, XRD	Detected C, O, Ni, Co, Mn, Cu, Al, F, P	No PSD; limited morphology-composition correlation
Garcia et al. [87]	NMC 18650	SEM, ICP-OES, TGA/DSC, PSD	Size-resolved chemical analysis of TR particulates	Poor resolution below 100 μm
Barone et al. [81]	NMC 18650	SEM-EDX	Nanoparticles, microspheres, and electrode fragments identified	No statistical PSD
Zhang et al. [80]	NMC 18650	SEM-EDX, PSD	Majority of particles were submicron; sulfur detected	Sample recovery may alter morphology
Grossetête et al. [88]	Prismatic NMC	SEM-EDX, laser PSD	Heterogeneous composition and broad PSD	Limited EDX statistics

2.6.5 Limitations and Gaps

Across the literature, several recurring methodological limitations constrain the comparability and completeness of particulate characterization during TR of LIBs. A major limitation is the lack of quantitative PSD analysis, particularly in the submicron regime, with many studies either focusing on broad size bins or omitting PSD entirely. In addition, particle morphology and chemical composition are often assessed using SEM-EDX, but typically in a qualitative or point-specific manner rather than statistically representative or spatially resolved mapping, limiting proper morphology–composition correlations. Sample preparation methods such as filtration, grinding, ultrasonication, and aqueous detachment of particles from substrates introduce further uncertainty by potentially altering the native size, aggregation state, or surface features of emitted particulates. Several studies also rely on filter-based aerosol collection rather than direct ejected powder sampling, which can bias the captured particle population toward finer aerosols and reduce

representativeness of bulk ejecta. Further inconsistency arises from the lack of a standardized definition of emitted particulates, with studies variously analyzing airborne aerosols, condensed deposits, ejected powders, or post-mortem electrode residues, which are not directly equivalent in either formation pathway or physical characteristics. Finally, many investigations are constrained by single-technique or single-condition analyses, limiting the ability to capture the coupled influence of TA, mechanical loading, and electrochemical state on particle generation. Collectively, these limitations highlight the need for an integrated and statistically sound approach that combines controlled particle collection with quantitative size distribution analysis and particle-resolved morphological and elemental characterization to enable direct correlation between particle size, morphology, and composition in TR ejecta.

The present work addresses several of these limitations by characterizing native TR-generated particles collected directly from NP-induced failure of an NMC 18650 cell. Quantitative PSD analysis was performed using SEM image segmentation, while morphology classification and EDX mapping enabled correlation of particle size, morphology, and elemental composition. The use of unground particles further preserved the native particle structure and agglomeration state generated during TR.

Acknowledgement:

Parts of the contents from chapters 1 and 2 are adapted from the published manuscript: A. S. Nair, X.Y. Wu, P. K. Das, and M. Fowler, "A Review of Nail Penetration and Thermal Abuse Tests of Lithium-Ion Batteries and Their Emission Characterization," *Batteries*, vol. 12, no. 2, p. 74, 2026, doi: 10.3390/batteries12020074.

Chapter 3 Nail Penetration Tests on LG-HG2 18650 NMC Cells

3.1 Overview

This chapter presents the results of nail penetration (NP) experiments conducted on LG-HG2 18650 (INR18650HG2) cylindrical LIB cells. The objective of the experiments were to investigate the influence of cell state of charge (SOC) and initial cell temperature on NP-induced thermal runaway (TR) behaviour. Attention was given to the resulting temperature response, ignition characteristics, and overall TR severity under different test conditions.

The chapter begins with a description of the experimental apparatus, instrumentation, and test procedures. This is followed by an investigation of the influence of SOC on TR behaviour, including a discussion of temperature evolution and event repeatability. Finally, the effects of low-temperature preconditioning on NP-induced TR are examined and compared with ambient-temperature results.

3.2 Test Chamber

The experimental apparatus consisted of a TOB 6047 Battery Crush and Nail Penetration Chamber manufactured by Xiamen TOB New Energy Technology Co., Ltd. The system is capable of performing both crush and NP tests on LIBs at controlled penetration speeds. Although the chamber is not vacuum sealed, it incorporates an explosion-proof enclosure designed to withstand the pressure rise and thermal hazards associated with battery TR. A photograph of the test chamber is shown in **Figure 4 (a)**.

(a)



(b)

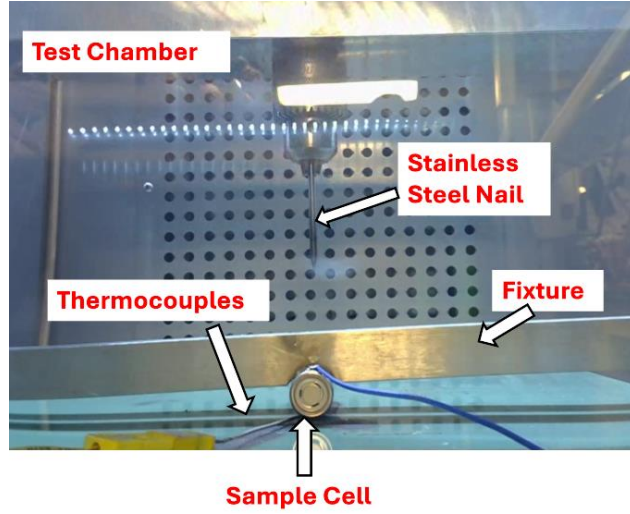


Figure 4: (a) TOB 6047 battery crush and nail penetration tester, (b) Explosion-proof chamber used for NP-induced TR experiments on lithium-ion cells

The chamber was equipped with a fixture designed specifically for cylindrical LIB cells and an insulating support plate to reduce heat transfer from the cell to the surrounding structure during testing. For NP experiments, a stainless-steel nail of 4 mm diameter was mounted using the chuck assembly shown in **Figure 4 (b)**. For crush testing, the chuck assembly can be removed and replaced with a flat compression plate.

To monitor the thermal response of the cell during NP, the chamber was instrumented with three K-type thermocouples positioned at strategic locations around the test specimen, as shown in **Figure 5 (a) and (b)**.

Thermocouple 1 (TC#1) was positioned in direct contact with the cell rupture plate, a critical failure location during TR events. The temperature recorded by this thermocouple is referred to as the surface temperature or T_s .

Thermocouple 2 (TC#2) was mounted on the nail chuck above the cell and positioned approximately 20 mm above the cell surface. This thermocouple was used to measure the temperature of the ejecta released during TR and is referred to as the ejecta temperature or T_{ej} .

Thermocouple 3 (TC#3) was installed along the emissions sampling line and was used to monitor the temperature of the gases transported to the sensor box. The temperature measured by this thermocouple is referred to as the emission temperature or T_{em} .

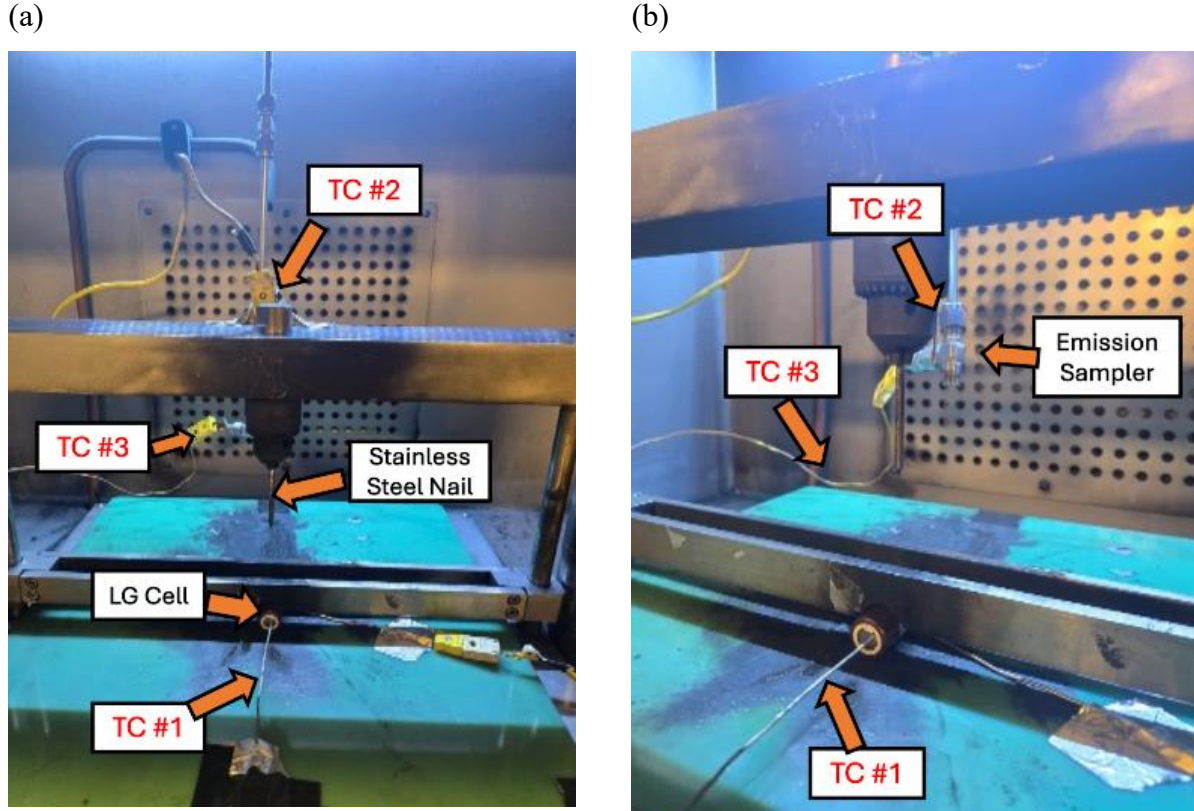


Figure 5: (a), (b) Instrumentation layout within the NP test chamber showing the locations of the surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}) thermocouples, together with the emissions sampling line

3.3 Cell Investigated

Commercially available LG-HG2 (INR18650HG2) cylindrical LIB cells were used mainly in this study. The cells measured open-circuit voltages ranging from approximately 3.60 to 3.65 V under nominal conditions. These cells are widely utilized in high-power applications such as power tools, making them representative of commercially relevant LIB technologies. The manufacturer specifications of the investigated cell are outlined in **Table 3**. The cell uses $\text{Li}[\text{NiMnCo}]\text{O}_2$ (NMC) as the cathode material 1, while its anode comprises a blend of graphite and silicon [89]. The

electrolyte contains three solvents: dimethyl carbonate (DMC), ethylene carbonate (EC) and propylene carbonate (PC) with LiPF₆ as the electrolytic salt [90]. The boiling points of DMC, EC, and PC are 90 °C, approximately 243–244 °C, and approximately 242 °C, respectively [91], [92], [93].

Table 3: Manufacturer specifications of the LG-HG2 (INR18650HG2) cylindrical lithium-ion cell investigated in this study [94]

Parameter	Value
Capacity	3 Ah
Nominal Voltage	3.6 V
Max. Charge Voltage	4.20 ± 0.05V
Max. Discharge Current	20 A
Max. Weight	47 g
Storage Temperature (1 month)	-20 to 60 °C
Cathode	Li[NiMnCo]O ₂ (NMC) [89]
Anode	Graphite + SiO [89]
Electrolyte	Dimethyl carbonate (DMC), ethylene carbonate (EC) and propylene carbonate (PC) + LiPF ₆ (salt) [90]

3.3.1 Cell Characterization and SOC Determination

Prior to NP, electrochemical characterization of the LG-HG2 cells was conducted using a MACCOR 4200 battery cycler to establish the voltage-capacity relationship of the investigated cells and determine the SOC corresponding to the selected preconditioning voltages.

The cells were first charged to 4.2 V using a constant-current constant-voltage (CC-CV) charging protocol and subsequently allowed to rest for one hour. Following the rest period, the cells were discharged incrementally at a constant current of 0.15 A, corresponding to approximately 0.05C based on the manufacturer's rated capacity of 3.0 Ah. Each discharge interval was maintained for one hour and followed by a one-hour rest period. This discharge-rest sequence was repeated until the cell reached a lower cut-off voltage of 2.0 V.

A low discharge rate was selected to minimize polarization and ohmic voltage losses, allowing the measured cell voltage to more closely represent the equilibrium voltage of the cell. Due to the incremental discharge protocol employed, the capacity recorded during each individual discharge step was accumulated to obtain the total discharged capacity removed from the cell. This cumulative discharge capacity was subsequently used to generate the voltage-capacity relationship shown in **Figure 6**.

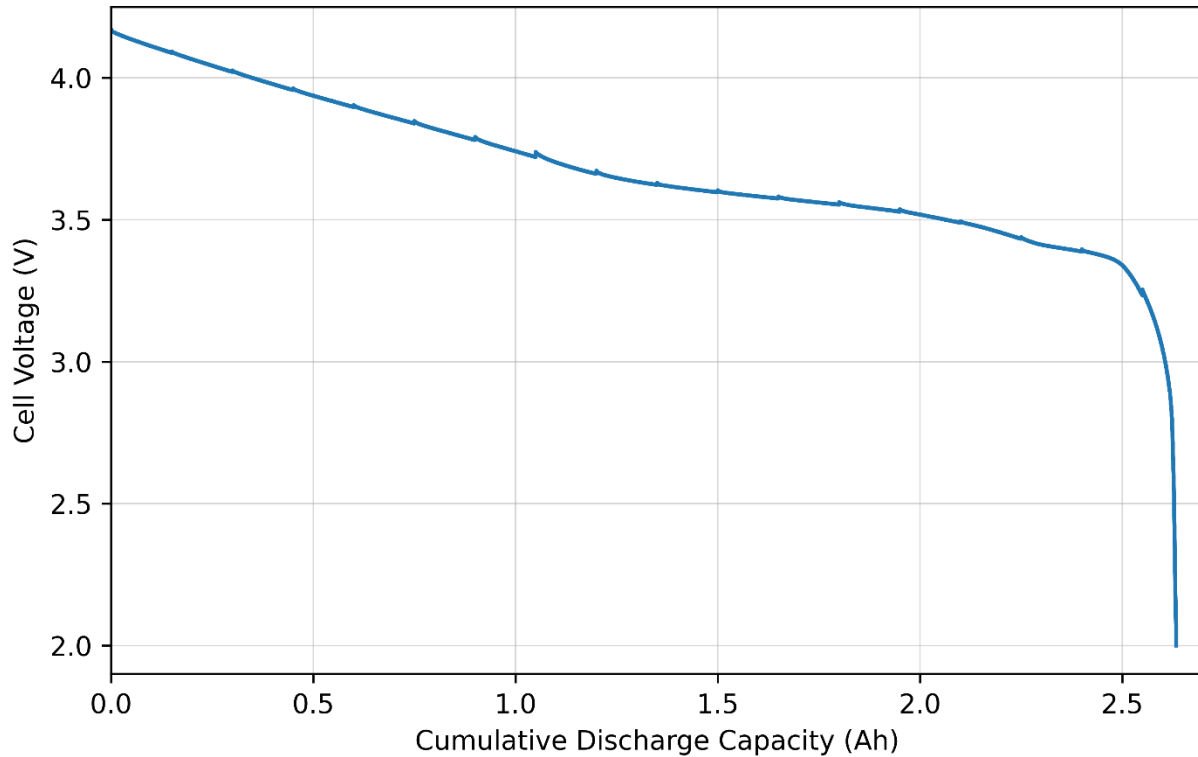


Figure 6: Voltage-capacity discharge curve of the LG-HG2 cell obtained using a 0.15 A (0.05C) incremental discharge protocol

The resulting discharge curve exhibits the characteristic behaviour of an aged LIB cell, consisting of an extended voltage plateau followed by a rapid decline in voltage as the cell approaches the lower cut-off voltage. The experimentally determined voltage-capacity relationship was used to estimate the SOC corresponding to the selected preconditioning voltages employed during the NP experiments.

The SOC was calculated using **Equation 1** as shown below.

$$SOC (\%) = 1 - \frac{Q_d}{Q_{max}} * 100\% \quad (1)$$

where Q_d is the cumulative discharged capacity and Q_{max} is the measured discharge capacity obtained from the characterization test.

Using the discharge curve shown in **Figure 6**, the selected preconditioning voltages of 4.2, 4.1, 3.9, and 3.8 V were found to correspond approximately to 100%, 95%, 77%, and 68% SOC, respectively. The resulting voltage-SOC relationship is summarized in **Table 4**. These voltage levels were subsequently used to investigate SOC influence on NP-induced TR.

Table 4: Voltage-SOC relationship for the LG-HG2 cell derived from the discharge curve shown in Figure 6

Preconditioning Voltage (V)	Estimated SOC (%)
4.2	100
4.1	95
3.9	77
3.8	68

3.4 Test Procedure

Prior to testing, the cells were preconditioned using the MACCOR 4200 battery cycler under constant-current constant-voltage (CC-CV) charging conditions. During charging, the cells were placed inside an environmental chamber to maintain controlled ambient conditions and provide an additional level of safety.

The same environmental chamber was used for low-temperature testing. To achieve the target cell temperatures, the cells were stored inside the chamber overnight prior to testing. NP experiments were conducted at four preconditioning voltages (4.2, 4.1, 3.9, and 3.8 V) and at various initial cell temperatures. The corresponding SOC values were determined from the voltage-capacity characterization described in Section 3.3.1. For low-temperature experiments, the cells were charged to 4.2 V and conditioned to -30 °C and -40 °C, respectively, representing temperatures below the manufacturer's recommended storage range.

Following preconditioning, the cell was secured within the test chamber beneath the penetration fixture. The temperature and gas sensing systems were activated prior to testing to establish baseline measurements. The penetration speed and nail displacement were controlled using the software. Penetration speed was set to 40 mm/s for all experiments. To investigate worst-case failure conditions, the nail was driven through the full diameter of the cell in every test. Following penetration, the nail stays in the final position for 20 seconds before retraction to the initial position.

The NP procedure used in this study was broadly consistent with commonly cited mechanical-abuse protocols, although it was not intended to reproduce a specific certification standard. As summarized by Patel et al. [95], GB/T 31485-2015 specified full penetration using a 5–8 mm steel nail at 25 ± 5 mm/s, whereas the cell-level procedure in SAE J2464 used a 3 mm nail at 80 mm/s. The present study used a 4 mm stainless-steel nail driven through the full cell diameter at 40 mm/s and held in position for 20 s. Thus, the selected nail diameter and penetration speed fall between these established procedures. Because nail geometry, speed, and retention time can influence the resulting internal short circuit and heat generation, these experiments should be considered comparative research tests rather than certification tests conducted in accordance with a particular standard.

A camera mounted on the chamber observation window was used to record the progression of TR. Data acquisition continued until the thermal event subsided and the measured cell temperature decreased below 60 °C.

Following completion of each test, the cell was removed from the chamber, and the chamber exhaust system was activated to purge residual gases. The damaged cells were subsequently isolated in sealed containers and stored in sand-filled buckets as a precautionary measure against delayed re-ignition.

Chapter 4 Results and Discussion

4.0 Overview

This section presents the effects of cell SOC and initial cell temperature on NP-induced TR behaviour. The discussion focuses primarily on the temperature responses measured by TC#1, TC#2, and TC#3, corresponding to the cell surface temperature (T_s), ejecta temperature (T_{ej}), and emissions temperature (T_{em}), respectively. The repeatability of the measurements is also assessed through an analysis of temperature variability between repeated tests.

4.1 Influence of SOC on Thermal Runaway

Cells tested at different SOC levels experienced significant differences in TR behaviour, indicating that SOC is a critical parameter influencing the severity and progression of NP-induced TR events.

4.1.1 Temperature Response

100 % SOC: Among the four investigated conditions, the fully charged cell exhibited the most severe TR response. Immediately following NP, ignition occurred at the penetration site, producing a plume of flaming ejecta as shown in **Figure 7 (a)**. This initial ejecta phase persisted for approximately 1 s before transitioning into a high-velocity jet flame emerging from the puncture location, as shown in **Figure 7 (b)**. During this stage, the rapid venting of gases generated an audible hissing sound, indicating the release of high-pressure decomposition products from within the cell.

As the TR event progressed, the jet flame gradually diminished and transitioned into a lower-intensity flame. Combustion continued for approximately 26 s before self-extinguishing, as shown in **Figure 7 (c)-(d)**. The complete TR event, from the onset of penetration to flame extinction, lasted approximately 28 s.

The observed severity of the TR event is attributed to the high energy content of the fully charged cell. At elevated SOC, a greater quantity of electrochemically stored energy is available to sustain exothermic decomposition reactions, resulting in more intense combustion and prolonged flame activity following cell rupture.

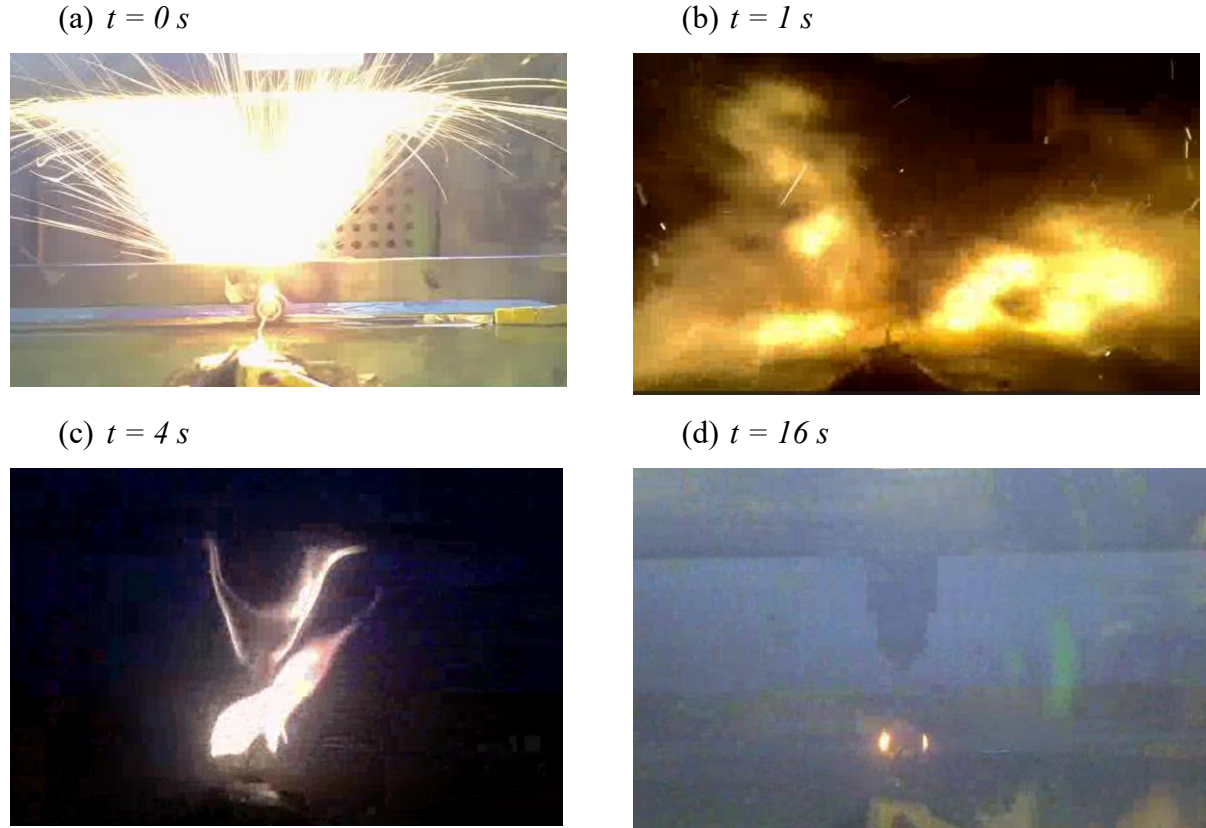


Figure 7: Progression of NP-induced TR in an LG-HG2 cell at 100% SOC. (a) Immediate ignition following penetration produced flaming ejecta, followed by (b) high-velocity flame ejection and (d) subsequent self-extinguishing combustion.

The corresponding temperature profiles are presented in **Figure 8**. The cell surface temperature T_s , measured at the rupture plate, showed the highest temperatures throughout the event and reached a peak value of $450 \text{ }^{\circ}\text{C}$ at $(t = 17) \text{ s}$. This temperature maximum occurred during the period of sustained combustion and indicates significant heat generation within the cell following rupture.

The ejecta temperature (T_{ej}), measured adjacent to the penetration site, reached a peak temperature of $194.6 \text{ }^{\circ}\text{C}$ at $(t = 9) \text{ s}$. Unlike T_s , the T_{ej} profile progressed to a secondary peak of $135 \text{ }^{\circ}\text{C}$ at $(t = 28) \text{ s}$. The first peak coincided with the primary flame ejection phase, whereas the second peak occurred near the end of the TR event, suggesting the continued release of hot gases or possible post-combustion reactions within the cell.

Following the temperature maxima, both T_s and T_{ej} gradually decreased as the cell cooled. The cell surface temperature remained above 60 °C for approximately 409 s (~7 min), while T_{ej} reached the same threshold after 335 s (~6 min). The emission temperature (T_{em}), measured along the gas sampling line, recorded substantially lower temperatures, reaching a maximum value of only 25 °C. This behaviour is attributed to heat losses along the sampling line and cooling of the gases prior to reaching the thermocouple location.

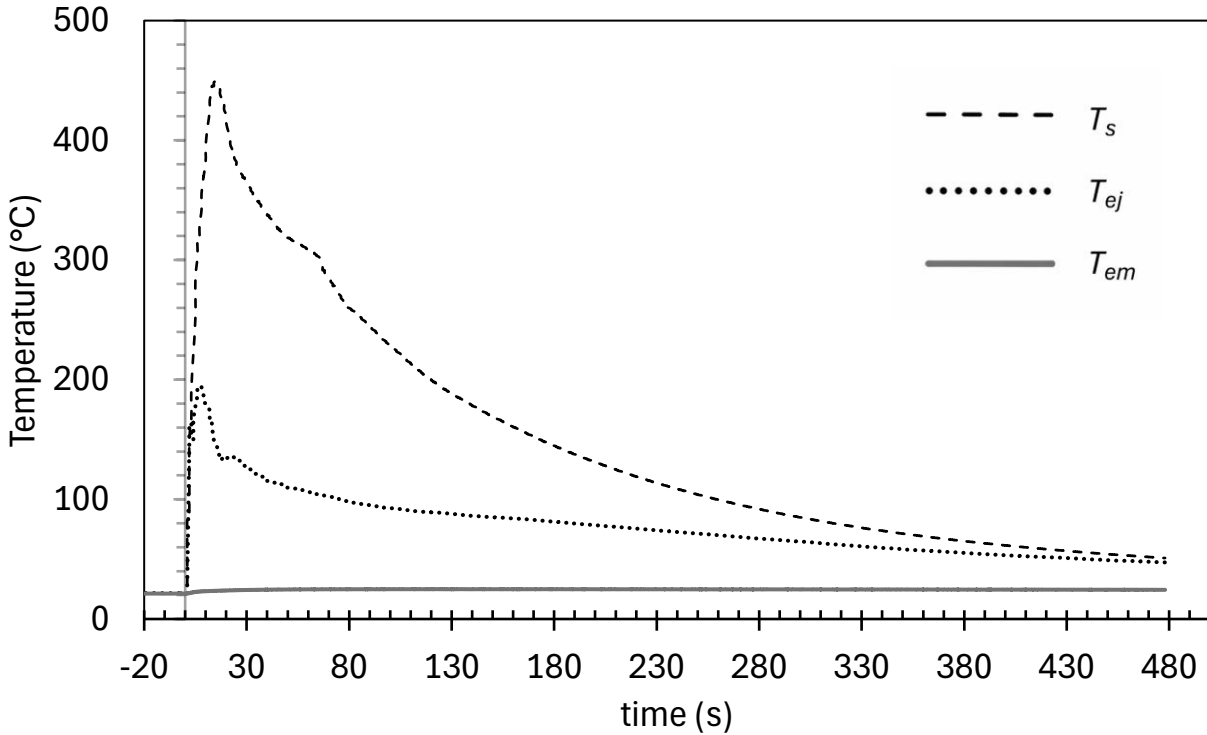


Figure 8: Temperature profiles obtained during NP-induced TR of an LG-HG2 cell at 100% SOC. Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}), are shown as a function of time

95 % SOC: The TR behaviour of the 95% SOC cell was comparable in severity to that observed for the 100% SOC case. Following NP, an initial ejecta phase was observed for approximately 2 s. Unlike the fully charged cell, however, this phase was followed by a brief pause of

approximately 1 s before the onset of a secondary, lower-intensity flame, as shown in **Figure 9 (a)-(c)**. This secondary flame persisted for approximately 48 s before self-extinguishing.

Visually, the flame intensity observed in the 95% SOC case was lower than that of the 100% SOC cell despite exhibiting a longer combustion duration. In addition, the flame spread over a larger portion of the test bed, suggesting that combustible material may have been deposited on the chamber surface during the initial venting process. As shown in **Figure 9 (a)**, the ejecta plume was directed laterally rather than vertically. This behaviour may have resulted from slight cell displacement during NP, leading to asymmetric venting from the penetration site.



Figure 9: Progression of NP-induced TR in an LG-HG2 cell at 95% SOC. Following the (a) initial ejecta phase, (b) a brief pause in visible combustion was observed before the onset of (c), (d) secondary flame

The corresponding temperature profiles are presented in **Figure 10**. Similar to the 100% SOC case, the cell surface temperature (T_s) recorded the highest temperatures throughout the event, reaching a maximum value of 415 °C. The ejecta temperature (T_{ej}) reached a peak value of 142 °C. Both

temperatures were lower than those recorded for the 100% SOC cell, indicating a reduction in thermal severity with decreasing SOC.

Interestingly, the brief pause observed visually between the initial ejecta phase and the subsequent flame was not reflected in the measured temperature profiles. Instead, both T_s and T_{ej} displayed a relatively continuous thermal response throughout the event. Following the temperature maxima, T_s decreased below 60 °C after approximately 376 s, while T_{ej} reached the same threshold after 186 s.

Unlike the 100% SOC case, the ejecta temperature profile showed a secondary temperature rise at approximately 303 s, reaching a maximum value of 58 °C before gradually decreasing. At this stage, visible flaming had already ceased, making it difficult to identify the origin of this temperature increase based solely on visual observations. Possible explanations include the delayed release of hot gases from within the cell or localized post-combustion reactions occurring near the thermocouple location.

The emission temperature (T_{em}) remained substantially lower than both T_s and T_{ej} , gradually increasing to a maximum value of approximately 25 °C during the TR event.

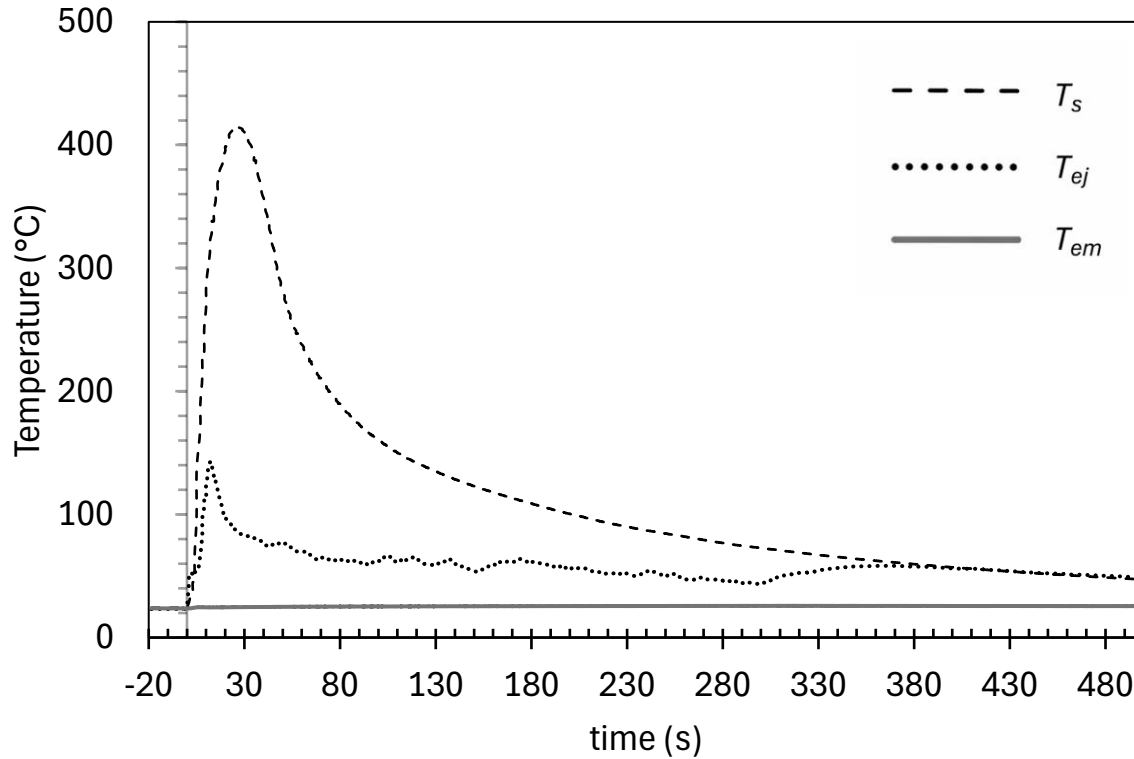


Figure 10: Temperature profiles obtained during NP-induced TR of an LG-HG2 cell at 95% SOC. Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}), are shown as a function of time

77 % SOC: The TR behaviour of the 77% SOC cell was generally similar to that observed for the 95% SOC case. However, unlike the latter, no noticeable pause was observed between the initial ejecta phase and the onset of secondary combustion. Following NP, the cell produced flaming ejecta that transitioned directly into sustained combustion. The overall combustion event lasted approximately 1 min 20 s from the onset of TR.

Although slight cell misalignment during penetration was observed as seen in **Figure 11 (a)**, the resulting flame remained localized near the penetration site and did not spread across the test bed as observed in the 95% SOC case. This suggests that the lateral flame spread observed previously may have been influenced by factors other than SOC alone, such as the direction of ejecta release and the deposition of combustible material during venting.

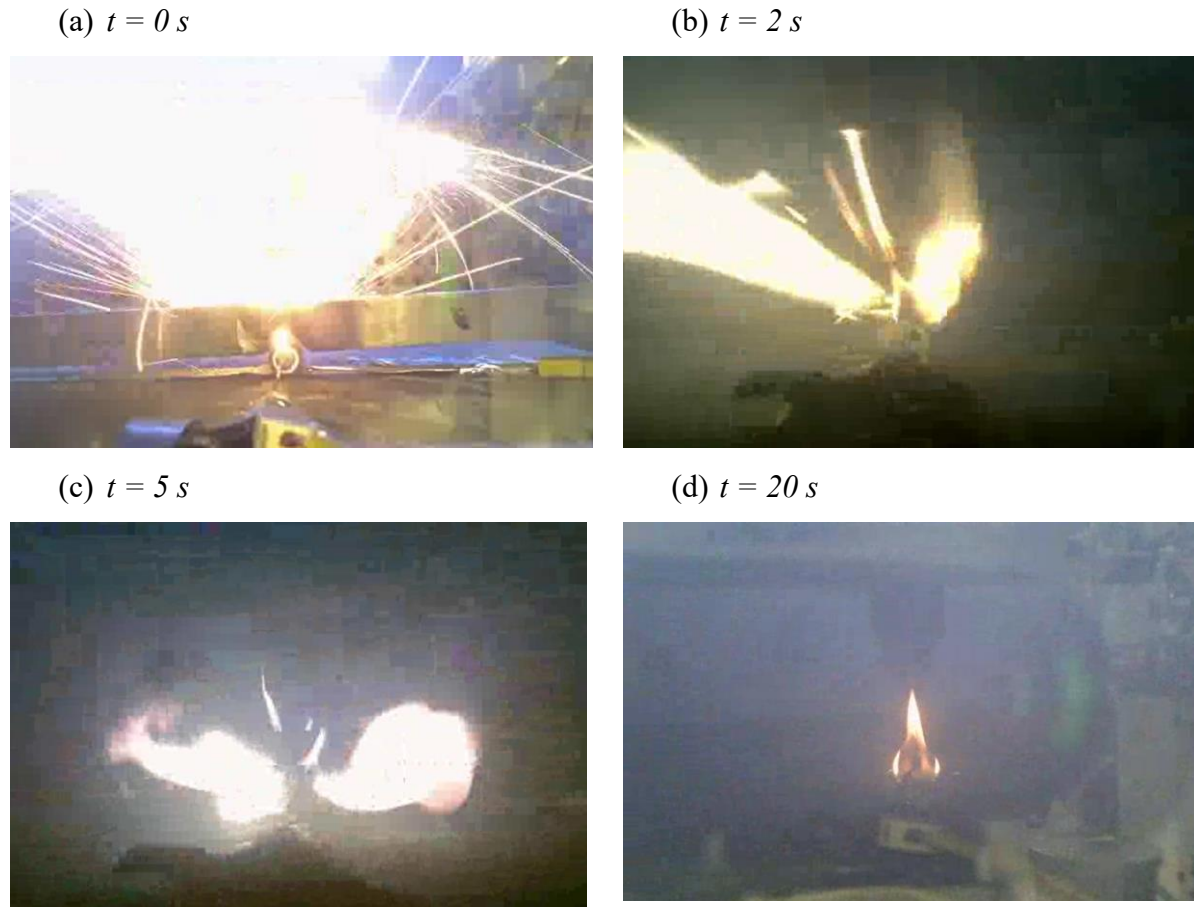


Figure 11: Progression of NP-induced TR in an LG-HG2 cell at 77% SOC. (a), (b), (c), (d) Continuous combustion was observed following penetration, with no distinct pause between the initial ejecta and secondary flame phases

The corresponding temperature profiles are shown in **Figure 12**. The cell surface temperature (T_s) reached a peak value of 481 °C, representing the highest temperature recorded among all tested SOC conditions. In addition to the elevated peak temperature, the T_s profile exhibited a broader, more parabolic shape than those observed for the 100% and 95% SOC cells, indicating that elevated temperatures were sustained for a longer duration during the first 100 s of the TR event. Following TR onset, T_s remained above 60 °C for approximately 647 s before cooling below this threshold.

The ejecta temperature (T_{ej}) had a markedly different response. Following an initial peak of 129.5 °C, the temperature decreased to a range of approximately 96–100 °C and remained relatively stable for nearly 1 min. This prolonged temperature plateau coincided with the sustained combustion phase observed visually. Thereafter, T_{ej} decreased to approximately 45 °C before exhibiting a secondary temperature rise to 68 °C. A similar behaviour was observed for the 95% SOC cell, although the secondary temperature rise occurred approximately 100 s earlier in the present case. Following this intermediate increase, the temperature profile transitioned into a gradual decay as the cell cooled.

The elevated T_s observed for the 77% SOC cell, despite its lower SOC relative to the 95% and 100% SOC cases, suggests that peak temperature alone may not be sufficient to characterize TR severity. Variations in venting behaviour, flame impingement on the thermocouple location, and local combustion conditions may also contribute to the measured temperature response.

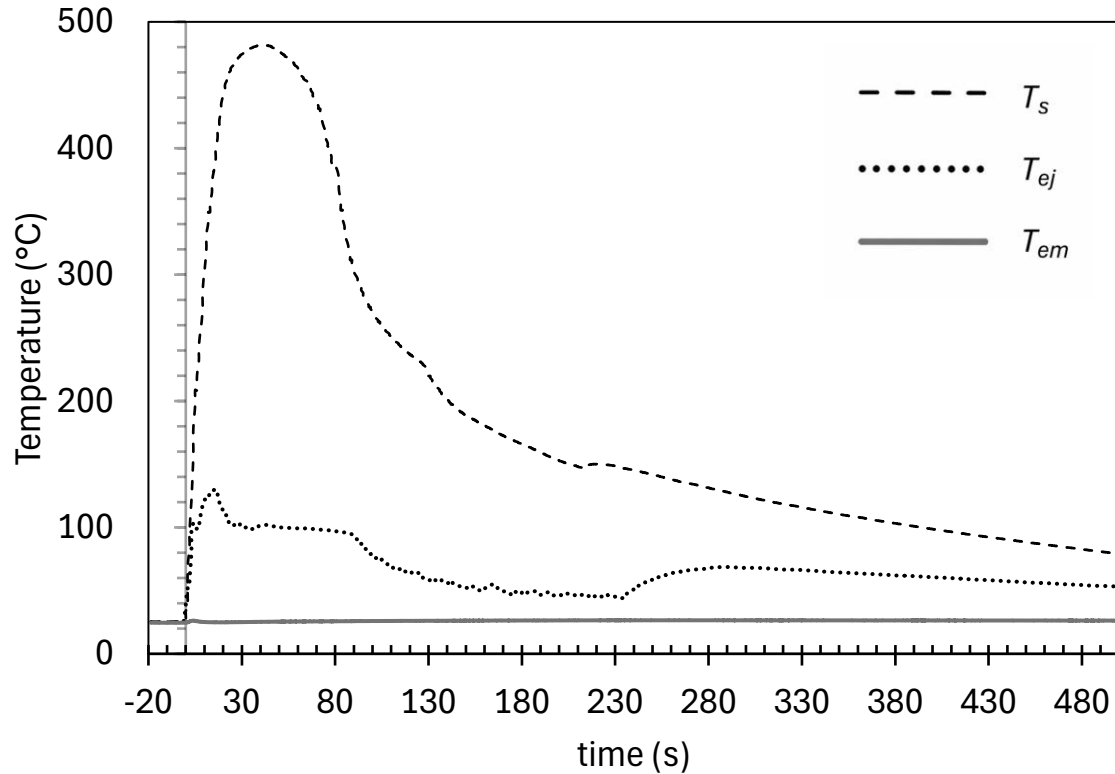


Figure 12: Temperature profiles obtained during NP-induced TR of an LG-HG2 cell at 77 % SOC. Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}), are shown as a function of time

68 % SOC: In contrast to the higher SOC conditions, no ignition was observed during NP of the 68% SOC cell. Although a substantial amount of smoke was released immediately following penetration, the event did not progress into sustained flaming combustion (**Figure 13**). This behaviour shows a significant reduction in TR severity relative to the 77%, 95%, and 100% SOC cases.

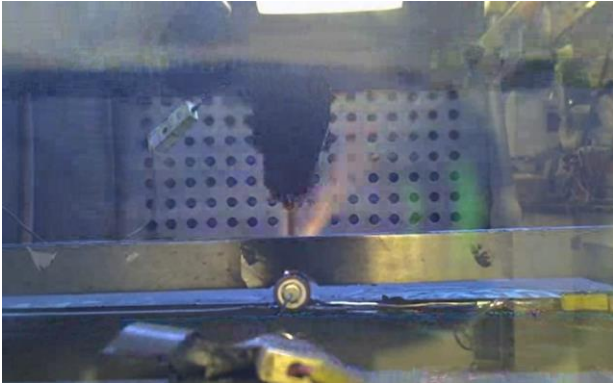
The smoke release was gradual and sustained throughout the event and was accompanied by a corresponding increase in the cell surface temperature (T_s) as shown in **Figure 14**. Unlike the higher SOC cells, which experienced rapid temperature increases associated with combustion, the T_s profile increased steadily, reaching a maximum temperature of 65 °C approximately 338 s (5.6 min) after the onset of TR.

The ejecta temperature (T_{ej}) exhibited only a modest thermal response. Immediately following penetration, the temperature increased from 24.5 °C to approximately 31 °C and remained near this value for roughly 100 s. Thereafter, T_{ej} gradually increased, reaching a maximum temperature of 38.6 °C at approximately 340 s after TR onset. The absence of sharp temperature peaks in both T_s and T_{ej} is consistent with the lack of visible combustion observed during the test.

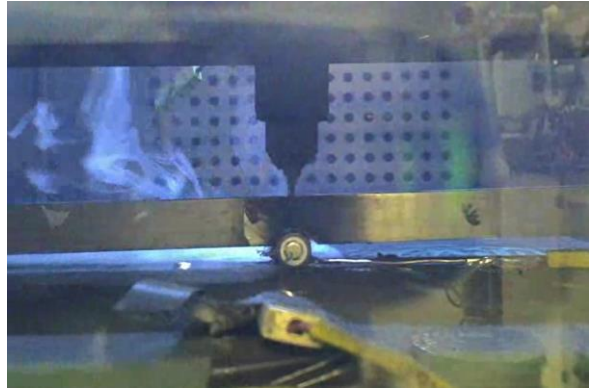
The emission temperature (T_{em}) remained largely unchanged throughout the experiment, exhibiting only a minor increase of approximately 1 °C following penetration. Compared with the higher SOC conditions, the substantially lower temperatures recorded at all three measurement locations indicate that the energy released during the event was insufficient to sustain ignition or significant combustion.

Overall, the results suggest that reducing the cell voltage to 3.8 V (approximately 68% SOC) markedly decreases the severity of NP-induced TR under the conditions investigated in this study. While venting and smoke generation were still observed, the absence of flaming combustion and the significantly lower temperatures distinguish this condition from the higher SOC cases.

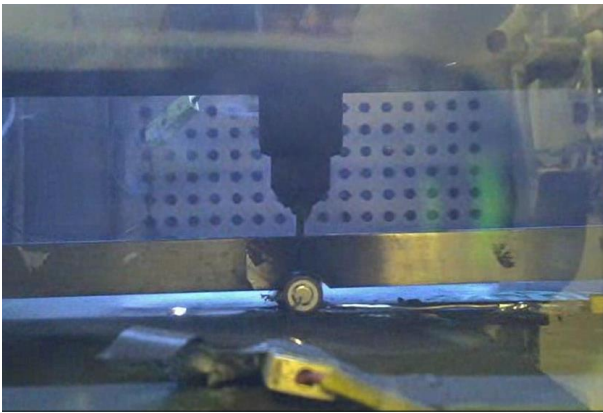
(a) $t = 0\text{ s}$



(b) $t = 2\text{ s}$



(c) $t = 10\text{ s}$



(d) $t = 20\text{ s}$

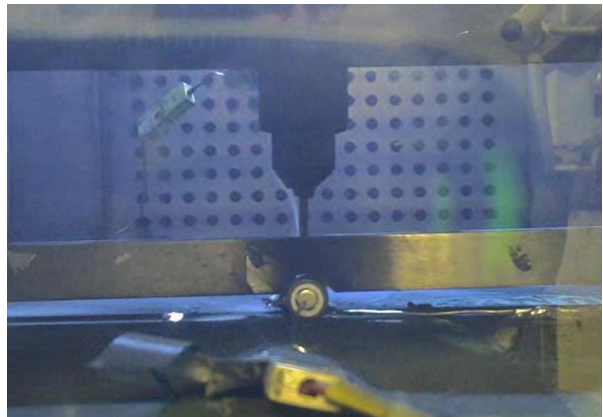


Figure 13: Progression of NP-induced TR in an LG-HG2 cell at 68% SOC. (a) No flaming combustion was observed following penetration; (b), (c), (d) the cell released a sustained plume of smoke throughout the event

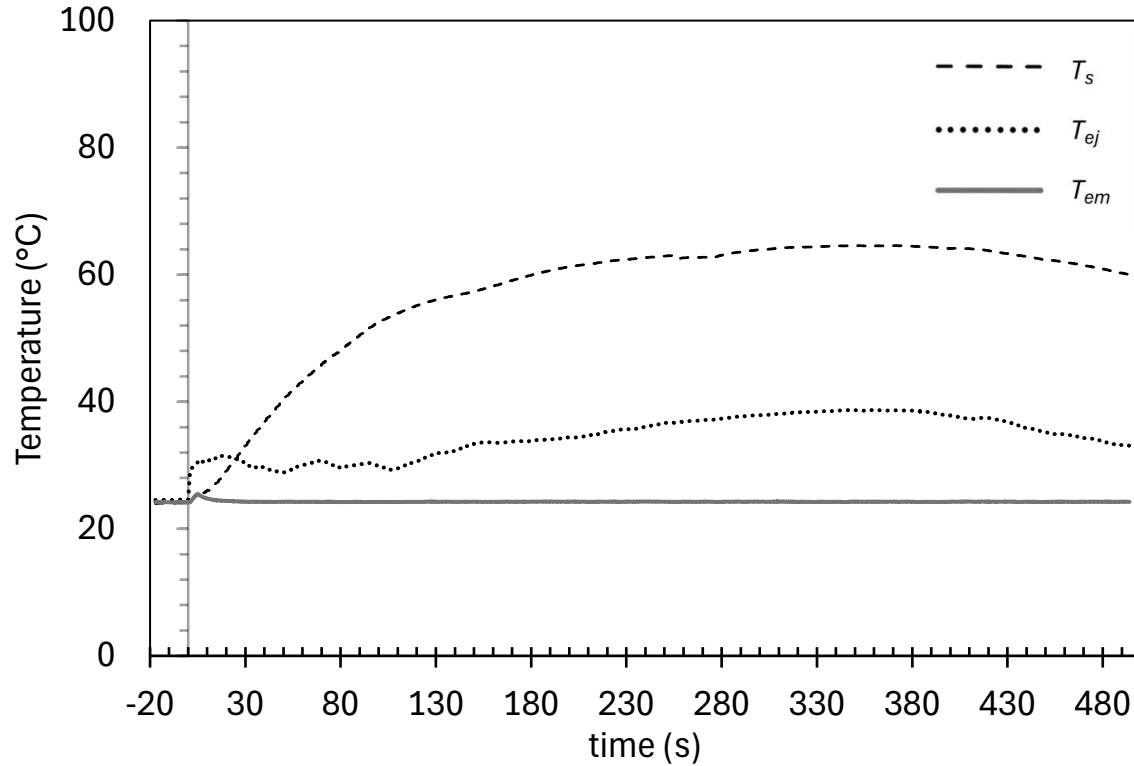


Figure 14: Temperature profiles obtained during NP-induced TR of an LG-HG2 cell at 68% SOC. Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}), are shown as a function of time

4.1.2 Discussion

Section 4.1.1 demonstrates that SOC strongly influences NP-induced TR behaviour. Cells tested between 77% and 100% SOC consistently underwent ignition, flaming combustion, elevated temperatures, and sustained heat release following NP. In contrast, the 68% SOC cell did not ignite and instead transitioned into gradual venting, smoke generation, and comparatively modest temperature increases. These observations suggest a strong dependence of TR behaviour on SOC, with a transition from combustive to non-combustive failure occurring between 68% and 77% SOC under the conditions investigated in this study.

Table 5 summarizes the key thermal characteristics obtained from the temperature-time profiles. The peak temperature represents the maximum temperature recorded by each thermocouple and provides an indication of event severity. The time to peak corresponds to the duration between TR

onset and the maximum recorded temperature, while the combustion duration represents the period of visible flaming. Cooling time is defined as the time required for the measured temperature to decrease below 60 °C. The maximum heating rate (dT/dt) represents the steepest temperature increase observed during the event and serves as an indicator of thermal escalation intensity.

Table 5: Comparison of characteristic thermal response parameters for NP-induced TR of LG-HG2 cells at 100%, 95%, 77%, and 68% SOC

SOC (%)	Temperature measured	Max. Temp (°C)	Time to Peak (s)	Combustion Duration (s)	Cooling Time (s) (T<60°C)	Max dT/dt (°C/s)
100	T_s	449.3	15	28	410	78.1
	T_{ej}	194.6	7		336	135.4
95	T_s	415.0	27	52	378	67.4
	T_{ej}	142.3	12		125	29.1
77	T_s	481.3	44	80	648	56.5
	T_{ej}	129.5	16		410	37.4
68	T_s	64.5	349	N/A	493	0.52
	T_{ej}	38.7	346		N/A	4.7

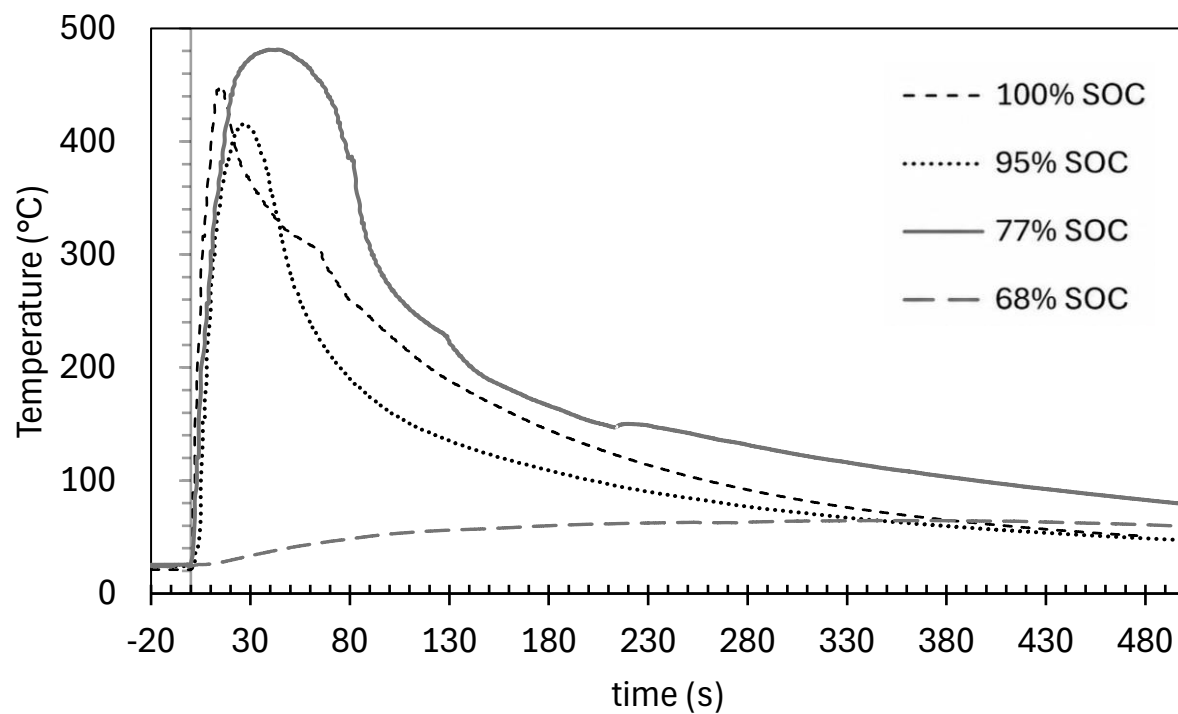


Figure 15: Comparison of representative surface temperature (T_s) profiles obtained during NP-induced TR of LG-HG2 cells at different SOC levels

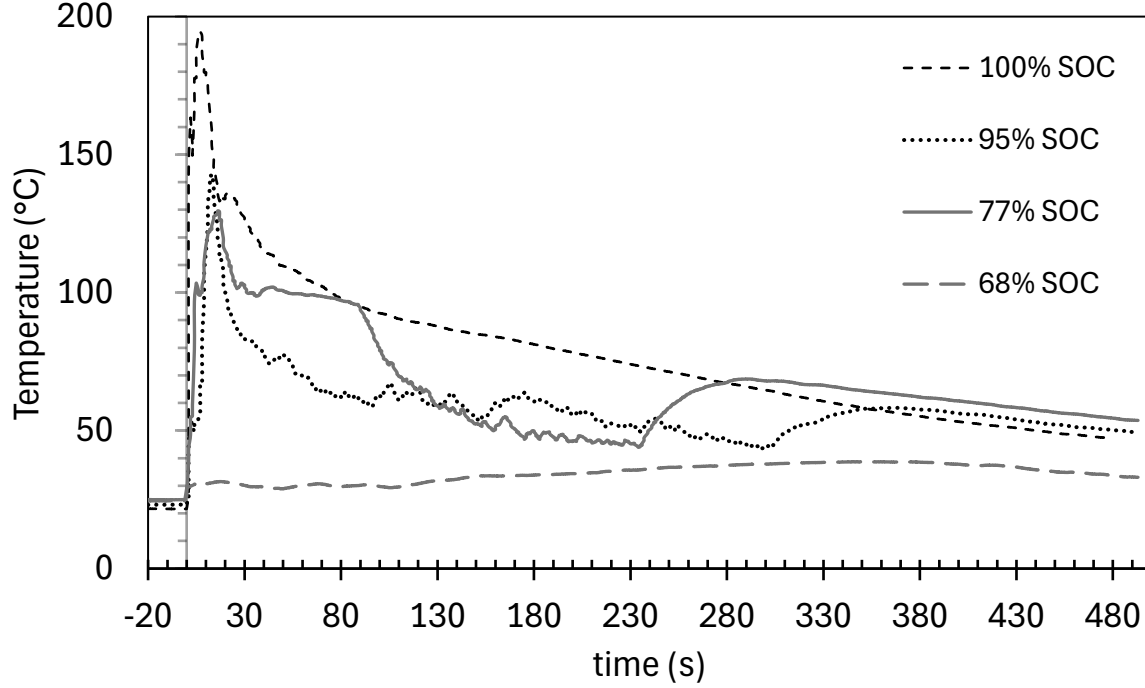


Figure 16: Comparison of representative ejecta temperature (T_{ej}) profiles obtained during NP-induced TR of LG-HG2 cells at different SOC levels

Analysis of the peak T_s values suggest no clear correlation between SOC and maximum cell surface temperature within the combustive SOC range (77–100%). Although higher SOC would generally be expected to produce higher temperatures, the highest measured T_s was observed at 77% SOC (481.3 °C), exceeding the peak temperatures recorded at both 95% SOC (415.0 °C) and 100% SOC (449.3 °C). This suggests that peak surface temperature alone is not a reliable indicator of TR severity and may be influenced by factors such as flame impingement, venting behaviour, and thermocouple location relative to the combustion zone.

In contrast, the peak ejecta temperature (T_{ej}) showed a more consistent relationship with SOC. The maximum T_{ej} increased from 129.5 °C at 77% SOC to 142.3 °C at 95% SOC and 194.6 °C at 100% SOC. This trend suggests that the temperature of the expelled gases and combustion products is more directly influenced by the amount of stored electrochemical energy within the cell. The substantially higher T_{ej} observed at 100% SOC is consistent with the violent ejecta and jet-flame behaviour observed visually during the test.

The time required to reach peak temperature increased with decreasing SOC for both thermocouples. For T_s , the time-to-peak increased from 15 s at 100% SOC to 27 s at 95% SOC and 44 s at 77% SOC. A similar trend was observed for T_{ej} , where the peak occurred at 7, 12, and 16 s for the 100%, 95%, and 77% SOC cases, respectively. At 68% SOC, the peak temperatures were reached only after approximately 340 s, indicating that the measured temperature rise was dominated by gradual heating of the surrounding environment rather than localized heat generation associated with combustion.

For the combustive cases, the duration of visible burning increased as SOC decreased from 100% to 77%. The fully charged cell burned for approximately 28 s, compared with 52 s at 95% SOC and 80 s at 77% SOC. This behaviour suggests that higher SOC conditions release energy more rapidly, producing intense but short-lived combustion events. Conversely, lower SOC conditions within the combustive regime appear to generate less violent but more prolonged burning.

Cooling behaviour differed between the two thermocouple locations. For T_s , the cooling time generally increased with increasing peak temperature and reflected the gradual dissipation of heat from the cell body. The post-peak decay profiles were relatively smooth and predictable. In contrast, T_{ej} exhibited more complex cooling characteristics, particularly for the 95% and 77% SOC cases. After the initial temperature decay, both cases progressed to a secondary temperature increase before returning to ambient conditions. Although no visible phenomena were observed during this stage, the behaviour may be associated with delayed release of hot gases, residual electrolyte reactions, or localized heating of material near the thermocouple. Interestingly, the secondary temperature rise occurred approximately 100 s earlier in the 77% SOC case than in the 95% SOC case. Additional experiments within this SOC range may help clarify the origin of this behaviour.

Unlike peak temperature, the maximum heating rate showed a clear positive correlation with SOC. For T_s , the maximum heating rate increased from 0.52 °C/s at 68% SOC to 56.5 °C/s at 77% SOC, 67.4 °C/s at 95% SOC, and 78.1 °C/s at 100% SOC. A similar trend was observed for T_{ej} , with the highest value occurring at 100% SOC (135.4 °C/s). The elevated heating rates at high SOC levels imply more rapid thermal escalation following NP and are consistent with the observed increase in flame intensity and ejecta violence. These results suggest that the rate of temperature rise is a more reliable indicator of TR severity than peak temperature alone.

Overall, the results indicate that SOC primarily influences the rate and mode of energy release during NP-induced TR rather than the absolute peak surface temperature. While peak T_s values exhibited significant variability among the combustive cases, ignition behaviour, heating rate, combustion characteristics, and overall thermal response all showed a clear dependence on SOC. The absence of ignition at 68% SOC further suggests the existence of a transition region below which the severity of NP-induced TR is substantially reduced.

4.1.3 Temperature Variability: Surface Temperature

The repeatability of the measured surface temperature profiles was assessed through repeated NP tests performed at each SOC condition. **Figure 17** presents the surface temperature (T_s) profiles obtained from the valid test repetitions. Due to thermocouple displacement during several experiments, complete temperature records were not available for all tests; therefore, only valid measurements are presented.

The T_s measurements showed good repeatability for the 100% and 95% SOC cases. In both conditions, the repeated tests produced comparable temperature profiles, with similar peak temperatures, time-to-peak behaviour, and post-peak cooling trends. This demonstrates that the surface thermocouple provided a reliable measurement of the cell thermal response for the higher SOC cases.

In contrast, greater variability was observed for the 77% and 68% SOC cases. For the 77% SOC condition, differences in peak temperature and the duration of elevated temperatures were observed between repeated tests. This suggests that, at intermediate SOC, the measured surface temperature may be more sensitive to local flame behaviour, venting direction, and thermocouple contact conditions. At 68% SOC, the overall temperatures remained substantially lower than those recorded for the combustive cases, but the relative variability between repeated tests was higher because the thermal response was occurred over a longer period.

Despite the variability observed at 77% and 68% SOC, the broader SOC-dependent trend remained consistent. The higher SOC cases produced rapid heating and elevated surface temperatures, whereas the 68% SOC case did not exhibit flaming combustion and remained at substantially lower temperatures. Therefore, while T_s provided repeatable measurements at 100% and 95% SOC, caution is required when interpreting variability at lower SOC conditions.

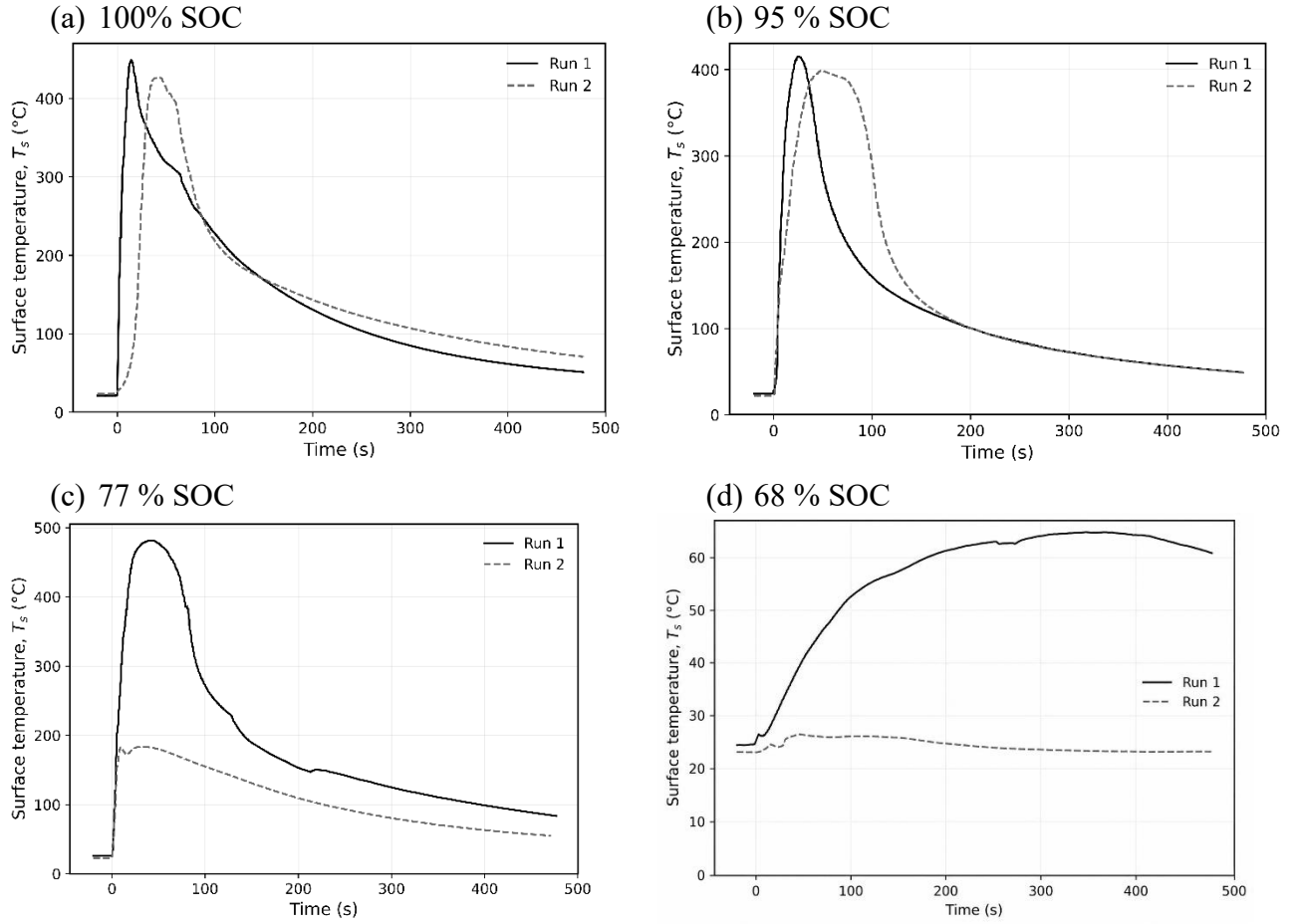


Figure 17: Surface temperature (T_s) profiles obtained from repeated NP tests of LG-HG2 cells at (a) 100% SOC, (b) 95% SOC, (c) 77% SOC, and (d) 68% SOC

4.1.4 Temperature Variability: Ejecta Temperature

Figure 18 presents the ejecta temperature profiles obtained during repeated NP tests. Compared with the T_s measurements, greater variability was observed in both the peak temperature and overall profile shape. This behaviour is expected because the T_{ej} thermocouple was positioned adjacent to the penetration site and is therefore highly sensitive to the direction of ejecta release, flame impingement, and local gas flow conditions.

Despite the increased variability, several common features were observed across repeated tests. For the combustive SOC conditions, the T_{ej} profiles generally entered a rapid temperature rise immediately following TR onset, followed by a gradual cooling phase. Secondary temperature

increases were also observed in some tests, suggesting that hot gas release or localized combustion may continue after the primary flame phase has subsided.

The greater variability in T_{ej} reflects the stochastic nature of venting and ejecta release during NP-induced TR. Small variations in cell positioning, penetration alignment, and flame trajectory can significantly influence whether the ejecta plume directly impinges on the thermocouple. As a result, local T_{ej} measurements may vary substantially between repeated tests even when the overall TR behaviour is similar.

These observations also highlight the importance of mechanical consistency in NP testing. A more robust test fixture that reduces cell displacement during penetration would likely improve the repeatability of ejecta direction and thermocouple exposure, thereby improving the reliability of T_{ej} measurements. This consideration is especially important for future studies aiming to quantify T_{ej} or compare ejecta behaviour across different cell conditions.

Although greater scatter was observed in the ejecta temperature measurements, the SOC-dependent response remained evident. Higher SOC tests generally produced more energetic ejecta and elevated temperatures compared with the 68% SOC case, which displayed only modest temperature increases and no sustained combustion. Thus, while T_{ej} is more sensitive to local experimental conditions than T_s , it remains a useful indicator of ejecta behaviour and TR severity.

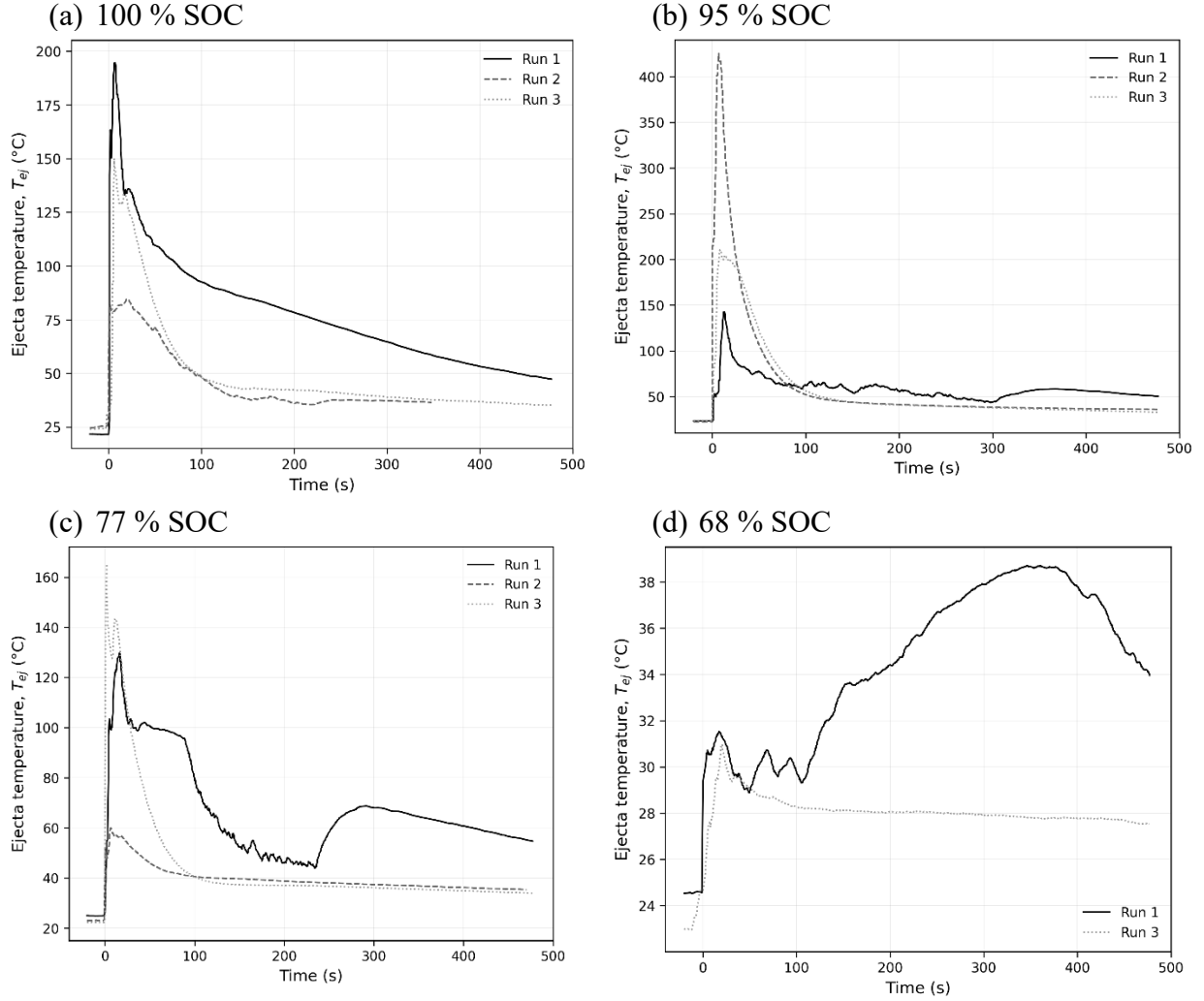


Figure 18: Ejecta temperature (T_{ej}) profiles obtained from repeated NP tests of LG-HG2 cells at (a) 100% SOC, (b) 95% SOC, (c) 77% SOC, and (d) 68% SOC

4.2 Influence of Cell Temperature on Thermal Runaway

To investigate the influence of low-temperature conditions on NP-induced TR, fully charged LG-HG2 cells were preconditioned at $-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$ for 24 h in an environmental chamber prior to testing. Immediately before testing, the cells were removed from the chamber and mounted on the NP fixture. Although the bulk cell temperatures corresponded to the chamber setpoints, the surface thermocouple (T_s) recorded temperatures of approximately $7\text{ }^{\circ}\text{C}$ and $1.3\text{ }^{\circ}\text{C}$ for the $-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$ cells, respectively. This discrepancy is attributed to the thermocouple configuration,

where only the probe tip was in direct contact with the rupture plate while the remainder of the thermocouple was exposed to ambient laboratory conditions.

Following removal from the chamber, the measured surface temperature gradually increased at approximately 0.02 °C/s due to heat transfer from the surroundings. The influence of these low-temperature conditions on TR behaviour is discussed in the following sections.

4.2.1 Temperature Response of Cells Preconditioned at -30 °C

Figure 19 and **Figure 20** present the results obtained from NP tests conducted on cells preconditioned to -30 °C. A total of two experimental runs were performed. In both cases, TR was initiated immediately upon NP, producing a plume of flaming ejecta without any observable delay. The initial ejecta phase was followed by a secondary flame that persisted for several seconds before self-extinguishing.

The overall TR behaviour was similar in both tests, and only minor differences were observed in the transition between the ejecta and secondary flame phases. One test had a brief temporal gap between these stages, whereas the second displayed a continuous combustion process. The total combustion duration ranged from approximately 38 to 44 s across the two experiments.

The corresponding temperature profiles are presented in **Figure 20**. Prior to NP, the measured surface temperature (T_s) was approximately 7 °C, whereas the ejecta temperature (T_{ej}) and emission temperature (T_{em}) remained near ambient conditions at approximately 23.5 °C. Following NP, T_{ej} experienced a rapid increase, reaching approximately 120 °C within 30 s of TR onset before decreasing rapidly thereafter.

In contrast, T_s increased more gradually and reached the highest recorded temperature among the three thermocouples, peaking at approximately 124 °C around 90 s after TR onset. Following the peak, T_s entered a gradual decline and decreased below 60 °C approximately 462 s after the initiation of TR. The emission temperature (T_{em}) remained comparatively unchanged throughout the event, increasing only slightly to approximately 25 °C.

Despite the reduced initial cell temperature, both tests underwent immediate TR following NP, indicating that preconditioning the cell to $-30\text{ }^{\circ}\text{C}$ was insufficient to suppress ignition under the conditions investigated in this study.

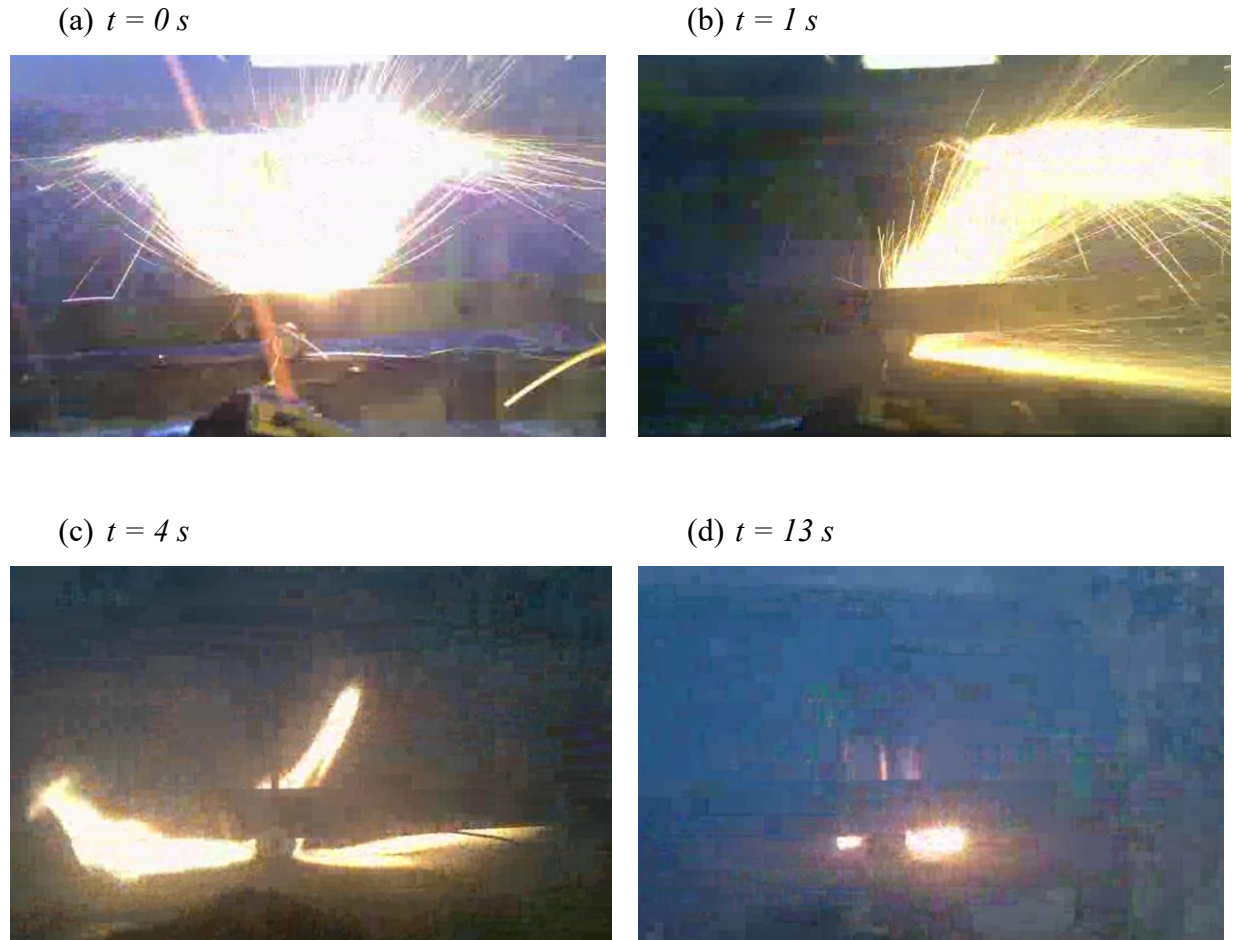


Figure 19: Progression of NP-induced TR in an LG-HG2 cell preconditioned to $-30\text{ }^{\circ}\text{C}$. (a), (b) Flaming ejecta was observed immediately following penetration and was followed by (c) secondary flame that persisted for several seconds before (d) self-extinguishing

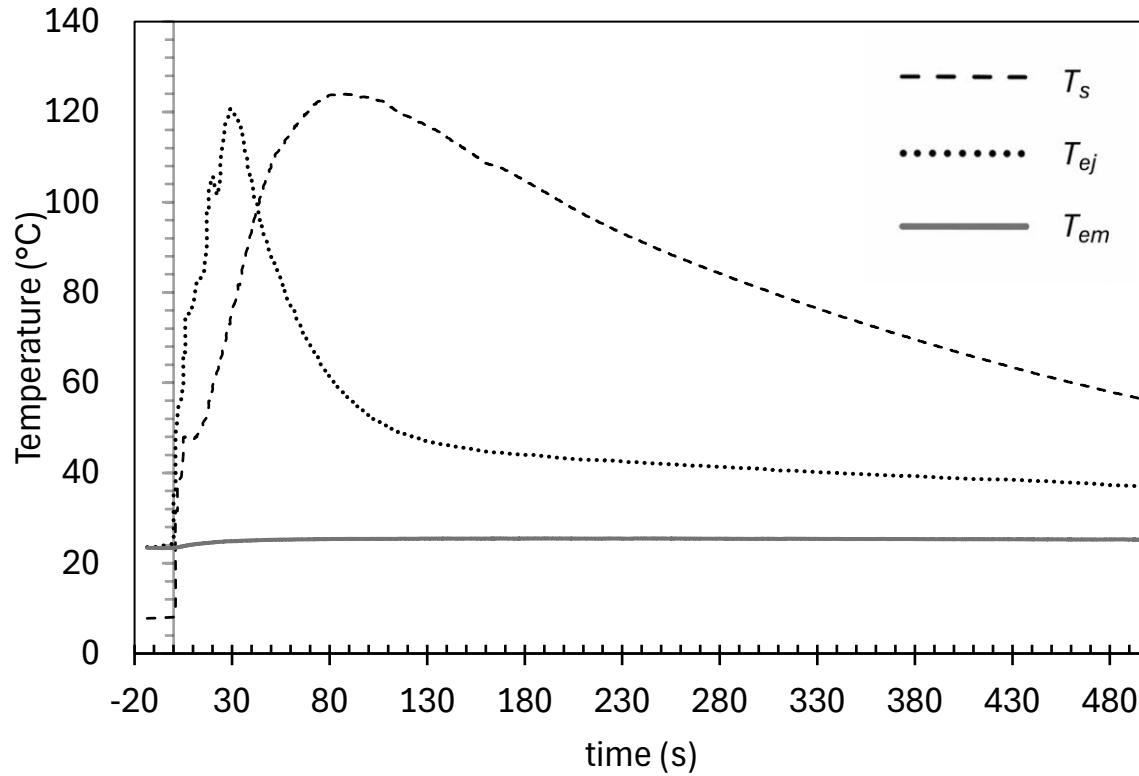


Figure 20: Temperature profiles of an LG-HG2 cell preconditioned to $-30\text{ }^{\circ}\text{C}$ during NP-induced TR. Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}) are shown as a function of time

4.2.2 Temperature Response of Cells Preconditioned at $-40\text{ }^{\circ}\text{C}$

Figure 21 to 26 presents the results obtained from NP tests conducted on cells preconditioned to $-40\text{ }^{\circ}\text{C}$. A total of three experimental runs were performed. Unlike the $-30\text{ }^{\circ}\text{C}$ tests, the cells exhibited two distinct TR behaviours following NP.

In the first and third experiments, TR was not initiated immediately upon penetration. Instead, a delay of approximately 20 s was observed between NP and the onset of visible combustion. In both cases, ignition occurred while the nail was being retracted from the cell. The resulting ejecta emerged from the rupture plate rather than the penetration site and was followed by a secondary low-intensity flame. The total duration of visible combustion ranged from approximately 46-60 s.

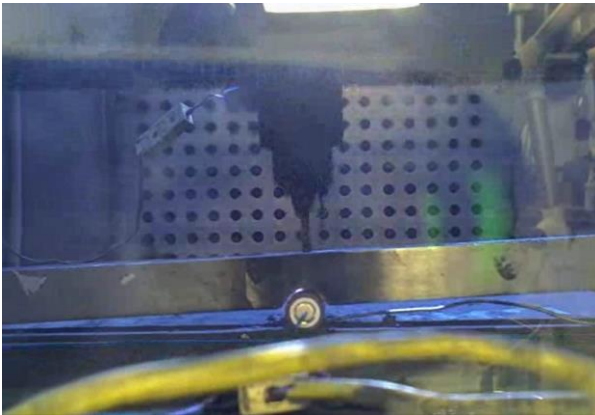
In contrast, the second test underwent immediate TR following NP. Flaming ejecta emerged directly from the penetration site, and the overall behaviour more closely resembled that observed during ambient-temperature experiments. Following a brief pause in combustion, a secondary flame developed and persisted for approximately 50 s before self-extinguishing.

The corresponding temperature profiles are presented in **Figure 22**, **Figure 24**, and **Figure 26**. In the first test, the measured surface temperature (T_s) increased gradually from 1.3 °C to approximately 11.3 °C during the 20 s delay period. Following ignition, T_s , rapidly increased to a peak value of 163.8 °C, while the ejecta temperature (T_{ej}) reached only 49 °C. In the second test, immediate ignition resulted in higher measured temperatures, with T_s , and T_{ej} , reaching peak values of 278 °C and 130 °C, respectively, within approximately 11 s of TR onset.

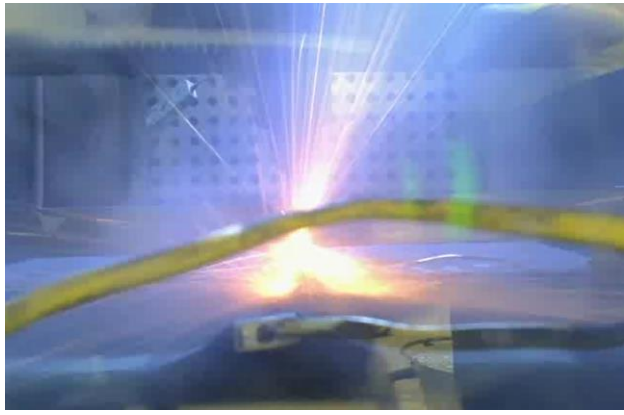
The third test experienced behaviour similar to that observed in the first experiment. Following NP, electrolyte leakage was observed from the penetration site before ignition occurred. After a brief flame event, the chamber filled with vent gases and reignition occurred approximately 13 s later. In this test, T_s , reached a peak temperature of approximately 460 °C, while T_{ej} , remained near 50 °C. Despite the differences in peak temperature, the overall progression of the event was consistent with the delayed-ignition behaviour observed in the first test.

Collectively, the results suggest that cells preconditioned to −40 °C exhibit greater variability in TR behaviour than those tested at −30 °C. Delayed ignition, rupture-plate venting, and electrolyte leakage were observed in multiple tests, suggesting that low-temperature conditions influence the progression of TR following NP.

(a) $t = 0\text{ s}$



(b) $t = 21\text{ s}$



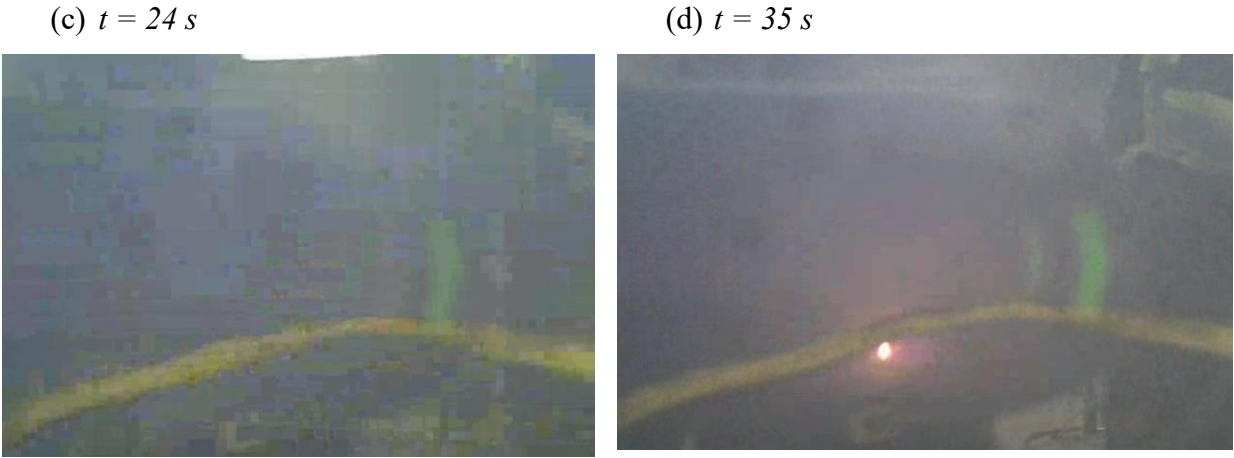


Figure 21: (a) Progression of NP-induced TR in an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ (Run 1). (b), (c), (d) Delayed ignition was observed following penetration, with ejecta emerging from the rupture plate during nail withdrawal

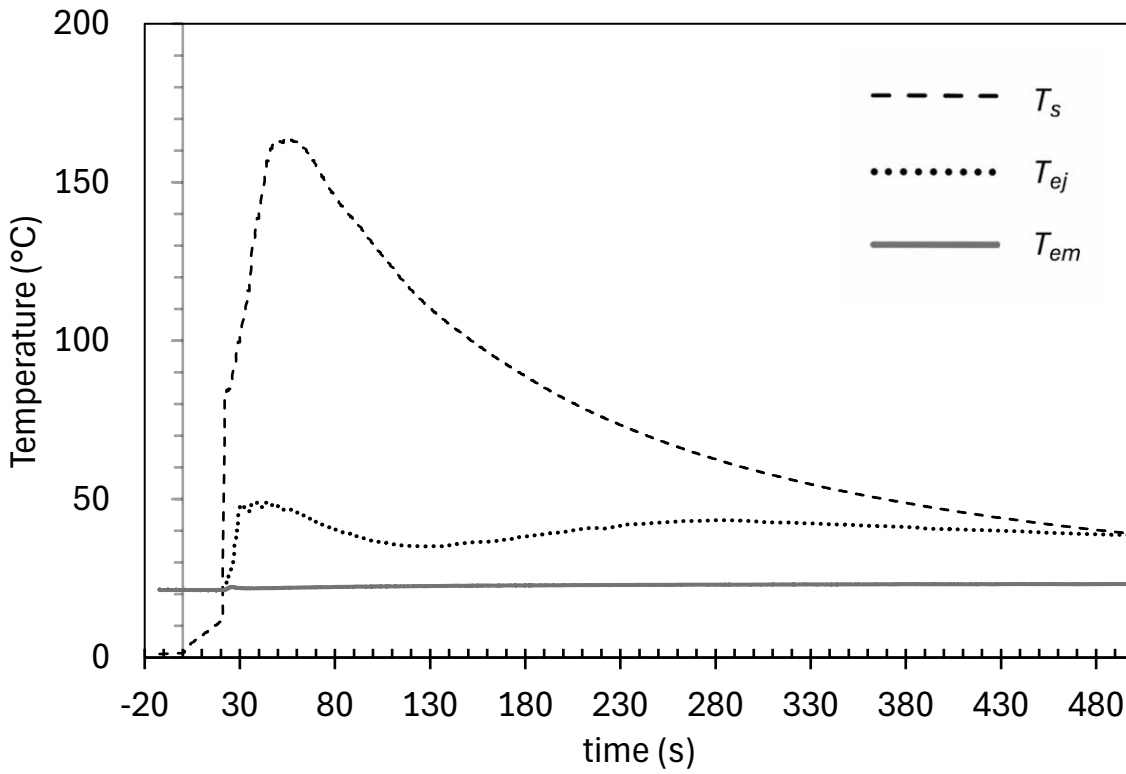


Figure 22: Temperature profiles of an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ during NP-induced TR (Run 1). Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}) are shown as a function of time



Figure 23: (a), (b), (c), (d) Progression of NP-induced TR in an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ (Run 2). TR was initiated immediately following penetration, producing flaming ejecta from the penetration site

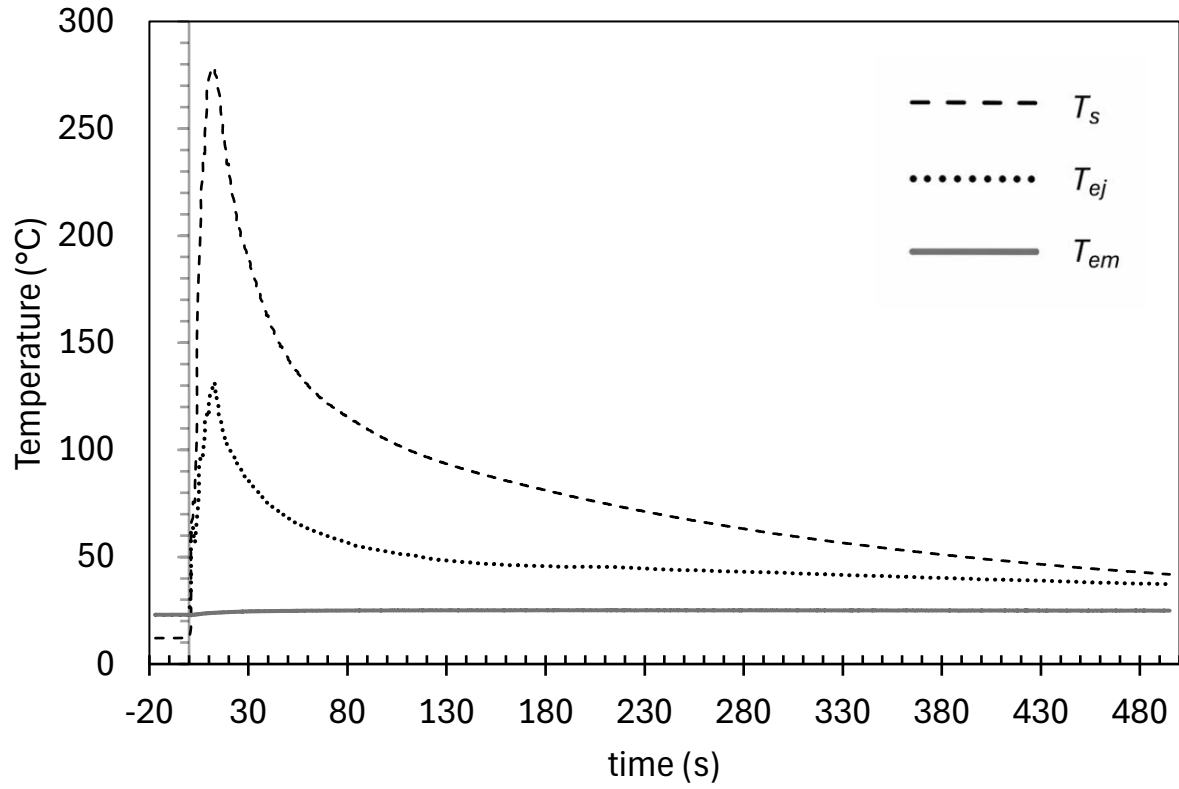
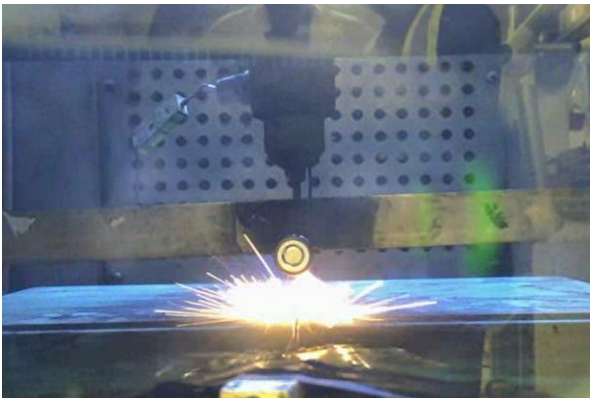
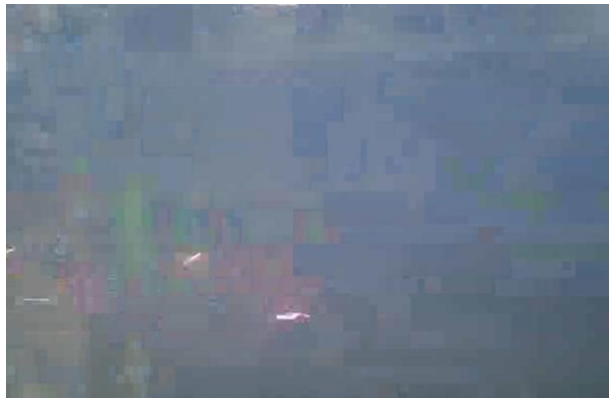


Figure 24: Temperature profiles of an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ during NP-induced TR (Run 2). Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}) are shown as a function of time

(a) $t = 0\text{ s}$



(b) $t = 2\text{ s}$



(c) $t = 13\text{ s}$



(d) $t = 60\text{ s}$



Figure 25: (a), (b), (c), (d) Progression of NP-induced TR in an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ (Run 3). Delayed ignition was observed following penetration, accompanied by electrolyte leakage from the penetration site prior to combustion

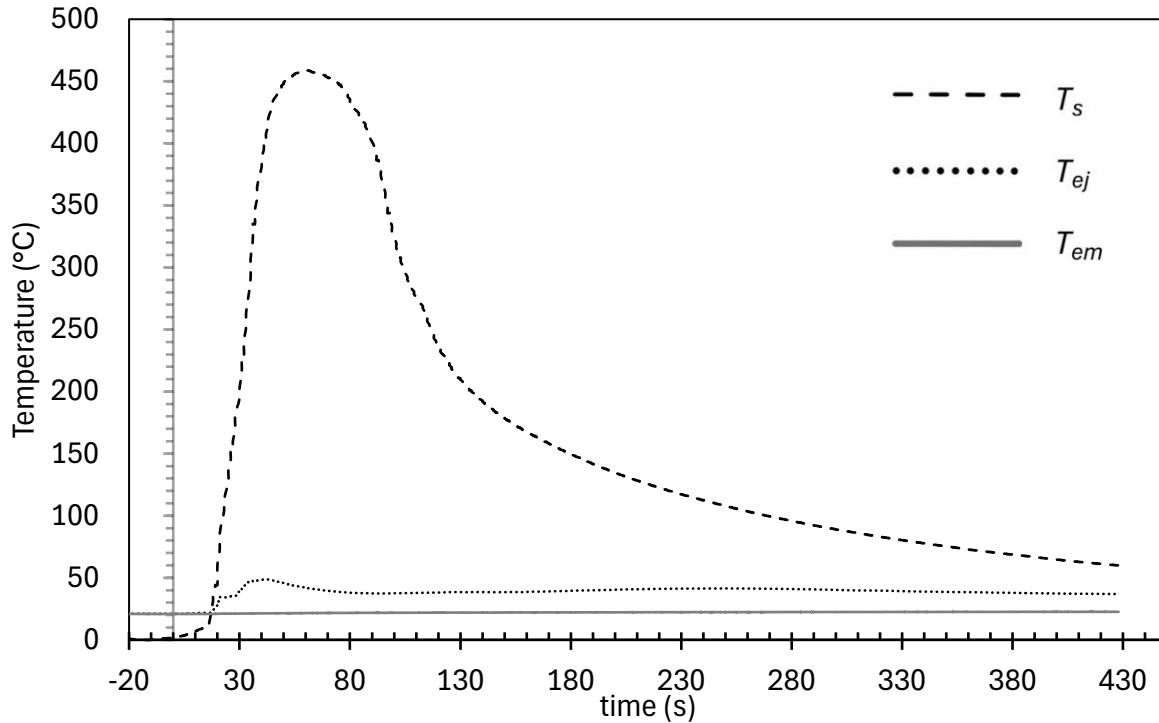


Figure 26: Temperature profiles of an LG-HG2 cell preconditioned to $-40\text{ }^{\circ}\text{C}$ during NP-induced TR (Run 3). Surface temperature (T_s), ejecta temperature (T_{ej}), and emission temperature (T_{em}) are shown as a function of time

4.2.3 Discussion

The results presented in Section 4.2.1 illustrate that the initial cell temperature influences the progression of NP-induced TR, although it does not necessarily prevent its occurrence. Cells preconditioned to $-30\text{ }^{\circ}\text{C}$ underwent immediate TR following NP in both experiments, indicating that reducing the cell temperature to this level was insufficient to suppress ignition. Despite the reduced initial temperature, the overall sequence of events, including ejecta release, flame formation, and subsequent cooling, remained similar to those observed under ambient conditions.

In contrast, cells preconditioned to $-40\text{ }^{\circ}\text{C}$ exhibited more complex behaviour. Two distinct TR responses were observed. In two of the three tests, ignition was delayed by approximately 20 s following NP and occurred while the nail was being retracted from the cell. Furthermore, the ejecta originated from the rupture plate rather than the penetration site. In the remaining test, TR occurred

immediately following NP and more closely resembled the behaviour observed under ambient conditions. These observations suggest that cooling the cell to $-40\text{ }^{\circ}\text{C}$ alters the mechanisms governing venting and ignition, resulting in increased variability in TR progression.

One possible explanation for the differing behaviour observed among the $-40\text{ }^{\circ}\text{C}$ tests is the temperature of the nail during penetration. The first and third experiments, both conducted using a nail at approximately room temperature, exhibited delayed ignition. In contrast, the second experiment, which was conducted shortly after the first test, the cell underwent immediate TR following penetration. It is possible that residual heating of the nail contributed to the earlier initiation of TR by locally increasing the temperature of materials surrounding the penetration site. However, because the nail temperature was not measured during testing, this explanation cannot be confirmed and should be regarded as a hypothesis rather than a definitive conclusion.

The observation of electrolyte leakage during the third $-40\text{ }^{\circ}\text{C}$ test further suggests that low-temperature conditions influence the venting behaviour of the cell. In this experiment, ignition appeared to occur after the electrolyte had exited the cell, indicating that combustible materials may accumulate outside the cell prior to ignition. This behaviour was not observed during the $-30\text{ }^{\circ}\text{C}$ tests and was less evident during ambient-temperature experiments. The delayed ignition and altered venting characteristics observed at $-40\text{ }^{\circ}\text{C}$ may therefore be associated with temperature-dependent changes in electrolyte transport, gas generation, or pressure release mechanisms within the cell.

Comparison of the measured temperatures further illustrates the limitations of using peak temperature alone as an indicator of TR severity. For example, the third $-40\text{ }^{\circ}\text{C}$ test produced the highest recorded T_s value among the cold-temperature experiments despite exhibiting delayed ignition. Visual observations revealed that the flame was directed toward the rupture plate, where the surface thermocouple was located. Consequently, the elevated T_s is likely attributable to local flame impingement rather than an increase in the overall severity of the TR event. Similar observations were made in the SOC study, where variations in flame direction and thermocouple exposure influenced the measured peak temperatures.

Overall, the results imply that reducing the initial cell temperature primarily affects the timing and mode of energy release during NP-induced TR rather than eliminating the possibility of TR altogether. While cells preconditioned to $-30\text{ }^{\circ}\text{C}$ behaved similarly to those tested under ambient

conditions, cells preconditioned to $-40\text{ }^{\circ}\text{C}$ experienced delayed ignition, altered venting locations, electrolyte leakage, and increased variability in TR progression. These findings suggest that low-temperature conditions modify the pathways leading to ignition and combustion but do not necessarily prevent TR following mechanical abuse.

4.2.4 Temperature Variability: Surface Temperature

Figure 27 presents the surface temperature (T_s) profiles obtained from repeated NP tests conducted on cells preconditioned to $-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$. Unlike the ambient-temperature SOC experiments, substantial run-to-run variability was observed under both cold-temperature conditions. Although all tests at $-30\text{ }^{\circ}\text{C}$ exhibited immediate TR following NP, the resulting temperature profiles differed considerably in both peak temperature and thermal evolution. Peak T_s values ranged from approximately $55\text{ }^{\circ}\text{C}$ to $491\text{ }^{\circ}\text{C}$, indicating that the measured surface temperature was strongly influenced by the progression of combustion and the interaction between the flame and thermocouple location.

The variability was further amplified for cells preconditioned to $-40\text{ }^{\circ}\text{C}$. Peak surface temperatures ranged from approximately $164\text{ }^{\circ}\text{C}$ to $459\text{ }^{\circ}\text{C}$ across the three tests. This variability is consistent with the differing TR behaviours observed during visual inspection, where delayed ignition occurred in two tests and immediate ignition occurred in the third. Consequently, the measured T_s profiles reflect both variations in heat release and differences in the location of combustion relative to the thermocouple.

These observations suggest that, under cold-temperature conditions, the variability in T_s is not solely attributable to measurement uncertainty but is also associated with genuine differences in TR progression between repeated tests.

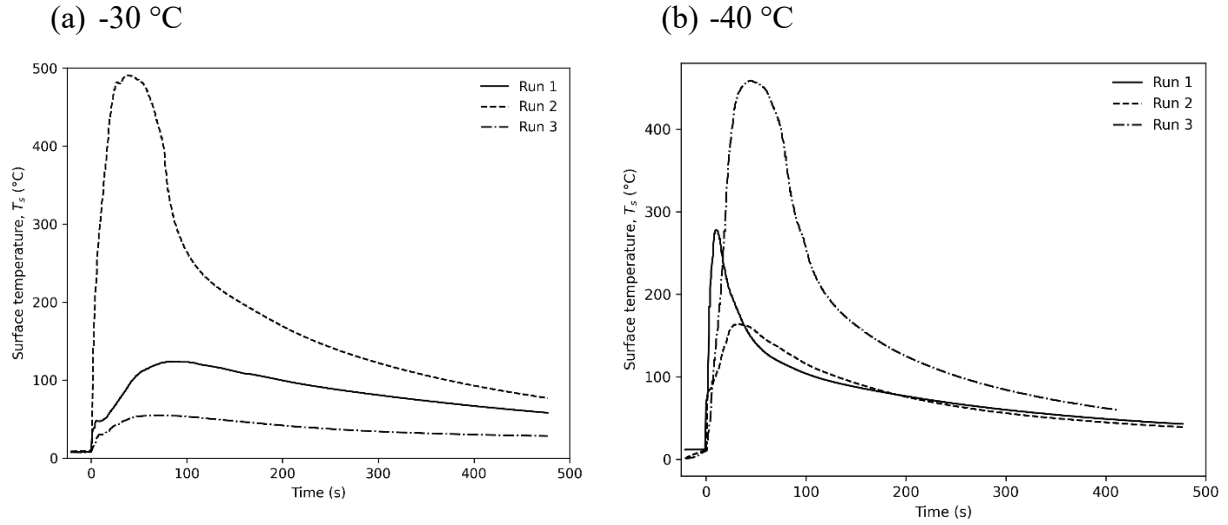


Figure 27: Surface temperature (T_s) profiles obtained from repeated NP tests of LG-HG2 cells preconditioned to (a) $-30\text{ }^{\circ}\text{C}$ and (b) $-40\text{ }^{\circ}\text{C}$

4.2.5 Temperature Variability: Ejecta Temperature

Figure 28 presents the ejecta temperature (T_{ej}) profiles obtained during repeated NP tests at $-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$. Compared with the surface temperature measurements, the ejecta temperatures showed lower variability for the $-30\text{ }^{\circ}\text{C}$ tests, with all three runs displaying similar temperature histories and peak temperatures between approximately $87\text{ }^{\circ}\text{C}$ and $140\text{ }^{\circ}\text{C}$. The overall shape of the temperature profiles was also relatively consistent, indicating comparable ejecta behaviour between repeated tests.

Greater variability was observed for the $-40\text{ }^{\circ}\text{C}$ condition. Two of the three tests produced peak ejecta temperatures of approximately $50\text{ }^{\circ}\text{C}$, whereas the remaining test reached approximately $130\text{ }^{\circ}\text{C}$. This behaviour is consistent with the visual observations described in Section 4.2.1, where two tests entered delayed ignition and one test underwent immediate TR following NP. The resulting differences in venting behaviour and flame trajectory directly influenced the temperature measured by the ejecta thermocouple.

Overall, the T_{ej} measurements show that cold-temperature conditioning increases the variability of ejecta behaviour during NP-induced TR. Nevertheless, the ejecta temperature measurements were

generally less sensitive to local flame impingement than the surface temperature measurements, resulting in somewhat more consistent trends across repeated tests.

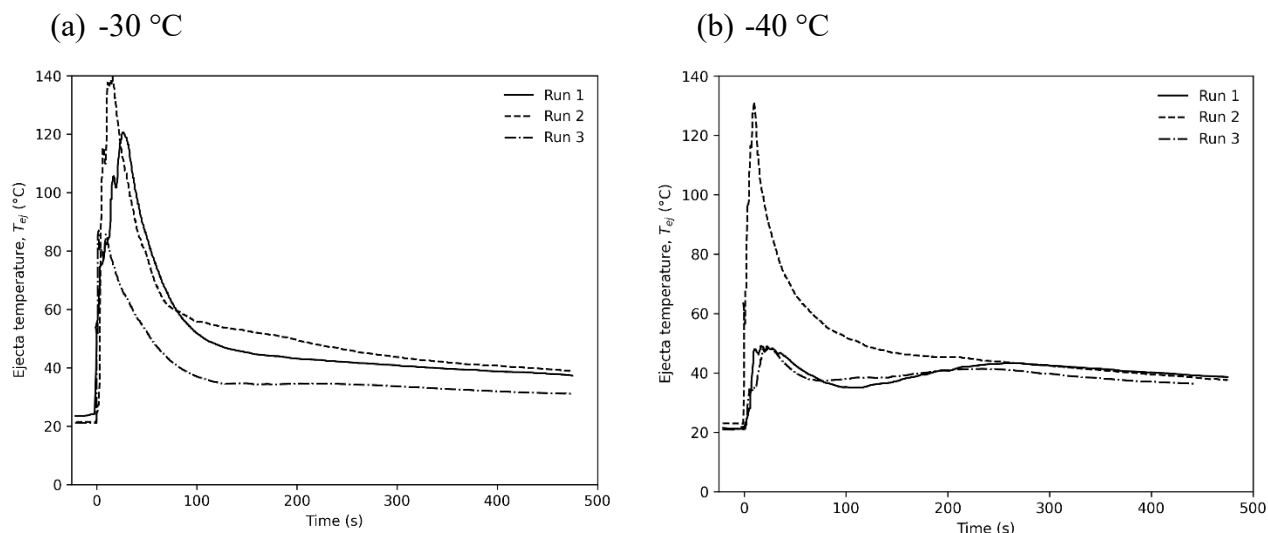


Figure 28: Ejecta temperature (T_{ej}) profiles obtained from repeated NP tests of LG-HG2 cells preconditioned to (a) $-30\text{ }^{\circ}\text{C}$ and (b) $-40\text{ }^{\circ}\text{C}$

4.3 Summary and Literature Comparison

In summary, it was found that NP testing of the cells preconditioned at low temperatures ($-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$) displayed reduced peak temperatures, ejecta temperatures (T_{ej}), and altered combustion behaviour. While TR was still observed under all low temperature conditions investigated, the severity and progress of the events were strongly influenced by cell temperature. Delayed ignition was observed in two of the three tests conducted at $-40\text{ }^{\circ}\text{C}$ whereas all $-30\text{ }^{\circ}\text{C}$ cells underwent immediate TR upon penetration.

The delayed ignition behaviour observed in the $-40\text{ }^{\circ}\text{C}$ cell is consistent with the findings reported by Böttcher et al. who conducted NP of NMC cells under low temperature conditions [96]. Their work suggested that reduced ionic conductivity within the electrolyte limits the electrochemical activity following mechanical damage, thereby suppressing heat generation and TR reactions at low temperatures. Similar conclusions were reported by Fang et al., who observed that electrolyte solidification occurring between approximately $-40\text{ }^{\circ}\text{C}$ and $-60\text{ }^{\circ}\text{C}$ resulted in a significant increase in internal resistance and a reduction in electrochemical activity during NP testing of

cryogenically treated NMC cells [97]. As temperature drops, the reduced mobility of lithium-ions restricts short-circuit current flow and slows the accumulation of heat required to trigger self-sustaining exothermic reactions. Consequently, although the internal short circuit generated by NP may still be present, the progression toward TR can be delayed due to the reduced rate of energy release. Similar mechanisms may explain the delayed ignition and reduced thermal response observed in the present study.

Similar observations were reported by Sunderlin et al., who performed NP tests on NMC 18650 cells at temperatures ranging from ambient conditions to cryogenic temperatures. They observed that cells penetrated at temperatures below approximately $-80\text{ }^{\circ}\text{C}$ displayed little immediate thermal response and remained largely inert following penetration. TR occurred only after the cells warmed to higher temperatures, with self-heating initiating near $-73\text{ }^{\circ}\text{C}$ and TR occurring at approximately $-23\text{ }^{\circ}\text{C}$ [98]. The authors attributed this delayed response to the suppression of electrochemical activity at low temperatures and the limited mobility of ions within the electrolyte, consistent with the mechanisms proposed by both [96] and [97]. Although the temperatures investigated in the present work were substantially higher than those employed by Sunderlin et al., the delayed ignition observed in the $-40\text{ }^{\circ}\text{C}$ tests in this work suggests that similar limitations of ionic -limited mechanisms may begin to influence TR progression at temperatures well above the electrolyte freezing regime.

The important observation from the present study is the difference in TR behaviour between $-30\text{ }^{\circ}\text{C}$ and $-40\text{ }^{\circ}\text{C}$. The increased variability between the two cases suggests that the temperature range might represent a transition region in which TR initiation becomes increasingly sensitive to local short circuit conditions.

Interestingly, Fang et al. reported that significant changes in battery electrochemical behaviour occurred when internal temperatures approached approximately $-60\text{ }^{\circ}\text{C}$ due to electrolyte solidification [97]. While the cells investigated in the present study were preconditioned to warmer temperatures, the delayed ignition at $-40\text{ }^{\circ}\text{C}$ suggests that the influence of temperature-dependent electrolyte limitations may begin well before complete electrolyte solidification occurs. The reduced peak temperatures observed on cells under low conditions further supports the hypothesis that the rate of heat generation was suppressed compared to ambient conditions. Although additional testing is required to establish a definitive threshold, the results indicate that low cell

temperatures can significantly influence the onset and progression of NP-induced TR even at temperatures higher than those investigated in cryogenic studies.

Overall, the low-temperature experiments demonstrate that reduced cell temperature does not eliminate TR following NP. Instead, low temperature conditions alter the progression of the failure by reducing reaction intensity and in some cases, delaying ignition. These findings highlight the importance of considering the dependence of temperature on electrolyte when evaluating battery safety under mechanical abuse conditions and reemphasize the importance of cell temperature in determining the severity and timing of TR events.

Chapter 5 Comparative Thermal Runaway Behaviour of Commercial Lithium-Ion Cells

5.1 Overview

This chapter presents a macroscopic comparison of NP-induced TR behaviour across commercially available LIBs of different chemistries, form factors, capacities, and SOC. Unlike Chapter 3 and 4, which provides a detailed investigation of LG-HG2 cells, the objective of this chapter is to compare the general failure characteristics exhibited by representative commercial cells during mechanical abuse.

The investigated cells include cylindrical and pouch cells of NMC, NCA, LMO, and LFP chemistries. The differences in ignition behaviour, flame propagation, venting location, combustion duration, peak temperatures, and the influence of SOC have been studied. These observations provide a broader understanding of how battery design influences NP-induced TR and establish context for the detailed particulate characterization presented in Chapter 6.

The cells investigated, and their corresponding test conditions are summarized in **Table 6**.

5.2 Cells Investigated

Table 6: Li-ion cell types investigated in this chapter

Cell Manufacturer	Chemistry	Form Factor	Cell Capacity	SOC Tested
Kokam Battery	NMC	Pouch	40 Ah	Nominal Voltage
Samsung Electronics	NMC	18650	2 Ah	Full SOC
Panasonic	NCA	18650	3.4 Ah	Full SOC, other SOC's
Efest Power	LMO	18650	2.6 Ah	Multiple SOC's
Samsung Electronics	NCA	21700	5 Ah	Multiple SOC's

5.3 Comparison of Thermal Runaway Behaviour

The NP experiments conducted on the investigated LIB cells revealed both common and cell-specific characteristics of TR. Although all cell types experienced internal short-circuit formation following penetration, the subsequent progression of TR depended strongly on cell chemistry, capacity, form factor, and SOC. Differences were observed in ignition behaviour, flame duration, combustion intensity, venting location, and the peak temperatures, indicating that the response of an LIB to mechanical abuse cannot be generalized across the different cell designs. **Table 7** shows the comparison of cell parameters and their respective TR characteristics observed during NP testing.

Cylindrical NMC cells generally underwent immediate TR with intense flame ejection and high peak temperatures. However, differences in venting behaviour were observed even among cells of similar chemistries. The Samsung INR-18650, and Samsung INR-21700 cells predominantly vented through the rupture plate, whereas the Panasonic NCR-18650B, LG-HG2-18650, and Efest IMR-18650 cells expelled combustion products directly from the penetration site. The Kokam pouch cell displayed markedly a very different behaviour, with delayed ignition occurring several minutes after penetration despite only limited initial heating.

SOC was found to be one of the most influencing parameters governing TR severity. Across all cylindrical cells investigated, higher SOC produced more severe combustion, greater peak temperatures, and fast ignition, whereas reducing SOC progressively suppressed TR. In contrast, differences in chemistry and cell geometry primarily influenced the location of venting, combustion duration, and overall flame characteristics.

The following sections compare the investigated cells with respect to their ignition behaviour, venting characteristics, the influence of chemistry and form factor, and the effect of SOC on NP-induced TR.

Table 7: Comparison of cell chemistry, design, and representative thermal runaway characteristics observed during nail penetration testing.

Cell	Chemistry	Form Factor	Capacity (Ah)	SOC	Venting Location	Peak Surface Temperature (°C)	Combustion Duration (s)	Lowest SOC Exhibiting TR	Remarks
LG-HG2 18650	NMC	Cylindrical (18650)	3.0	100, 95, 77, 68%	Penetration site	481	28–80*	77%	TR severity strongly dependent on SOC; sustained smoke only at 68% SOC
Samsung INR18650	NMC	Cylindrical (18650)	2.0	100%	Rupture plate	434	17	—	Immediate voltage collapse following NP
Panasonic NCR18650B	NCA	Cylindrical (18650)	3.4	100, 90, 70, 50%	Penetration site	545	~60	90%	Smoke generation only at 70% SOC and below
Efest IMR18650	LMO	Cylindrical (18650)	2.6	100, 80, 70, 50%	Penetration site	550	~40	70%	Sparks and smoke observed at 50% SOC
Samsung INR21700	NCA	Cylindrical (21700)	5.0	100–90, 70, 40%	Rupture plate	~800	~60	70%	Cell remained visibly red-hot for ~1 min following flame extinction
Kokam	NMC	Pouch	40	Nominal voltage	Penetration site	235†	~780 (13 min)	Not investigated	Delayed ignition several minutes after NP

Notes:

- Combustion duration of the LG-HG2 cell varied with SOC, increasing from approximately 28 s at 100% SOC to approximately 80 s at 77% SOC.
- Peak temperature recorded for the Kokam pouch cell is likely underestimated because the thermocouples were being removed prior to delayed ignition.

5.3.1 Ignition Characteristics

The ignition behaviour of the investigated LIBs showed considerable variation following NP, despite all cells undergoing mechanical deformation and internal short-circuit formation. Three distinct ignition modes were observed: (i) immediate TR accompanied by flaming combustion, (ii)

delayed ignition following an initial smoke release, and (iii) smoke generation without sustained combustion. The occurrence of each mode depended primarily on the cell SOC, chemistry, and design.

Immediate TR was the predominant response among the cylindrical cells investigated. The LG-HG2, Samsung INR18650, Panasonic NCR18650, Efest IMR18650, and Samsung INR21700 cells all ignited immediately when tested at sufficiently high SOC's. The TR sequences for these cells are presented in **Figure 29-32**. In each case, NP was followed almost instantaneously by venting of high-temperature gases and PM, which subsequently ignited to produce sustained flaming combustion. Although the overall sequence of events was similar, noticeable differences were observed in flame propagation, combustion duration, and the location from which the ejecta was expelled.

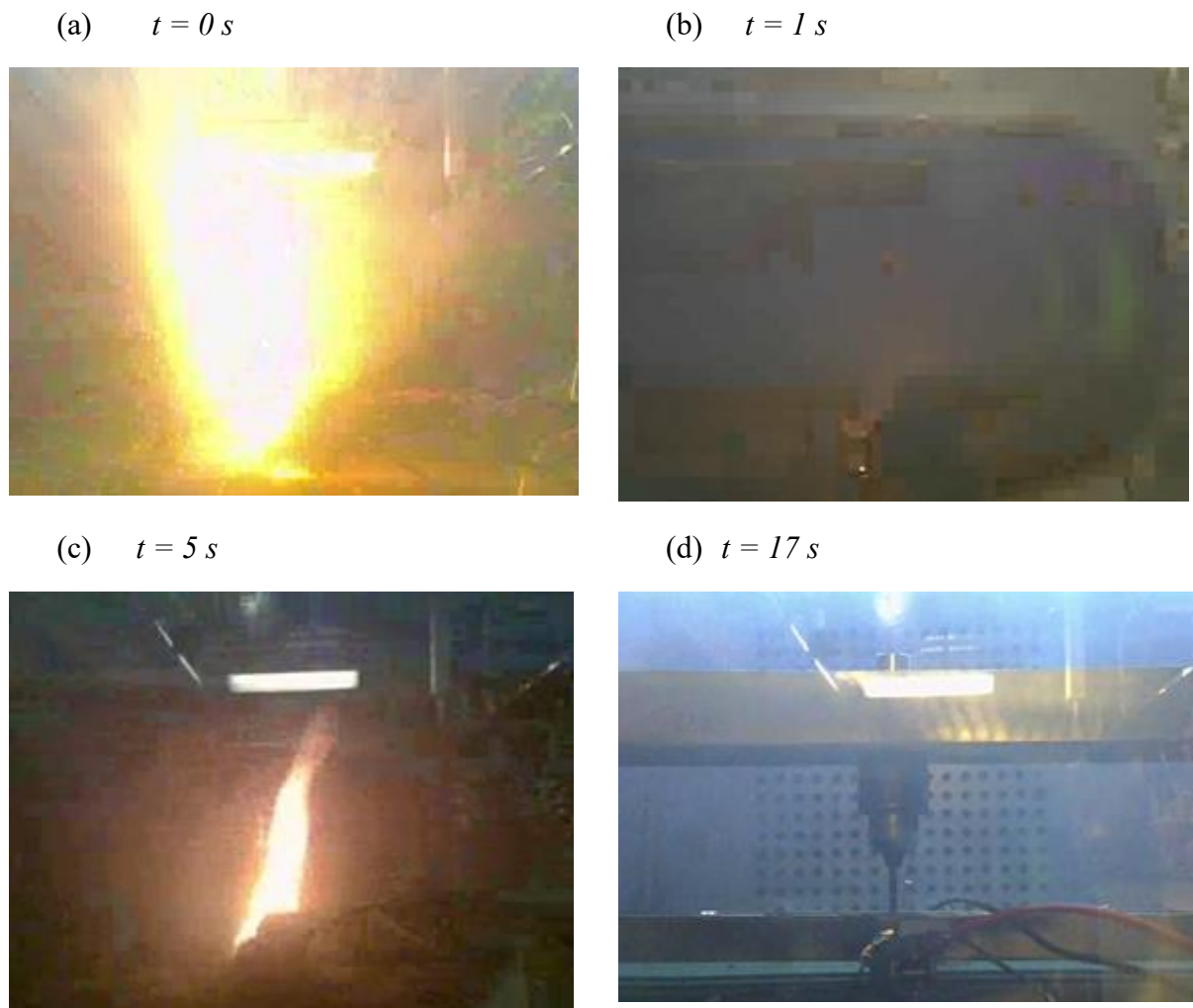


Figure 29: Sequence of NP-induced TR of the Samsung INR18650 (NMC) 18650 cell at 100% SOC: (a) venting and flame ejection from the rupture plate ($t = 0$ s), (b) brief pause in visible combustion, (c) secondary flaming combustion ($t = 5$ s), and (d) complete flame extinction ($t = 17$ s)

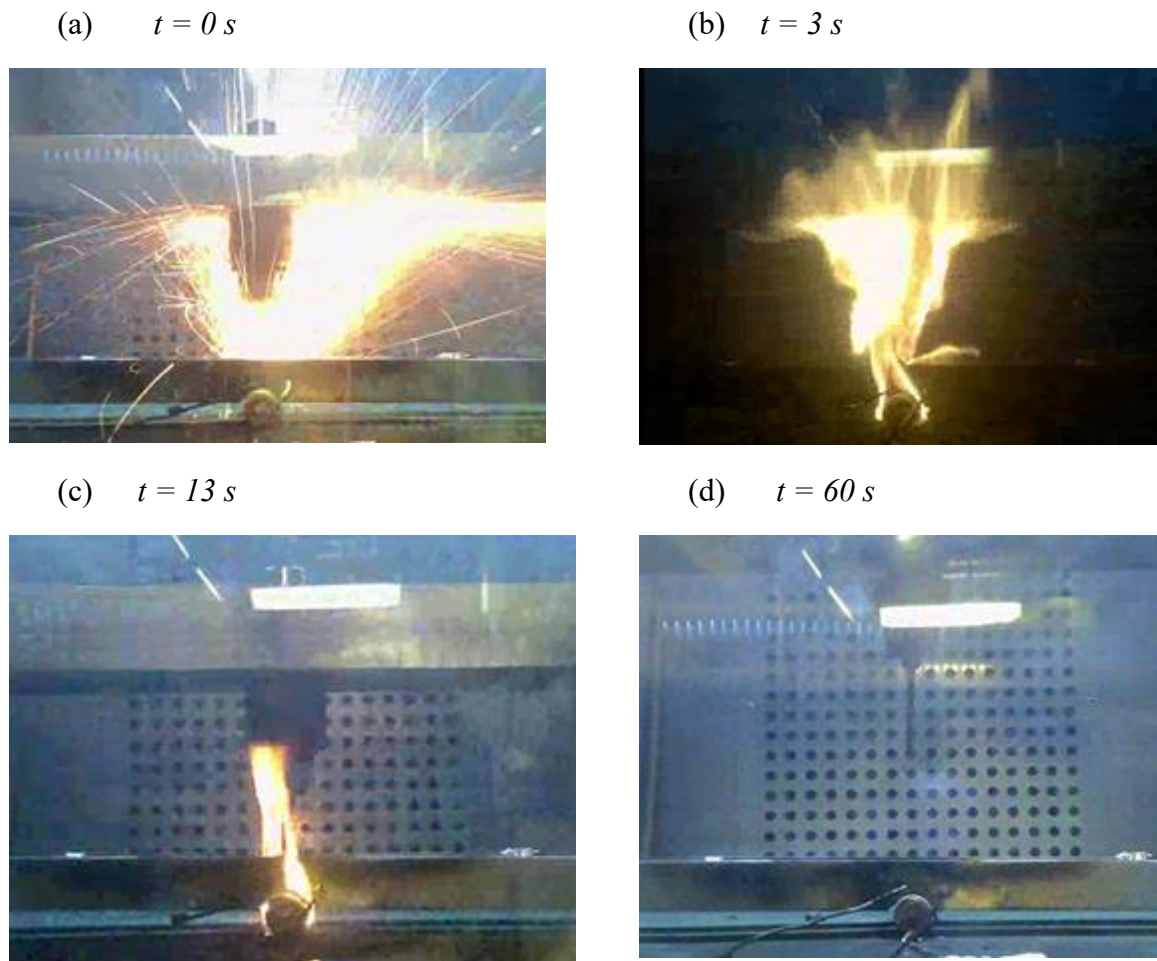


Figure 30: Sequence of NP-induced TR of the Panasonic NCR18650B (NCA) 18650 cell at 100% SOC: (a) venting and flame ejection from the penetration site ($t = 0$ s), (b) and (c) continued combustion, (d) complete flame extinction ($t = 60$ s)

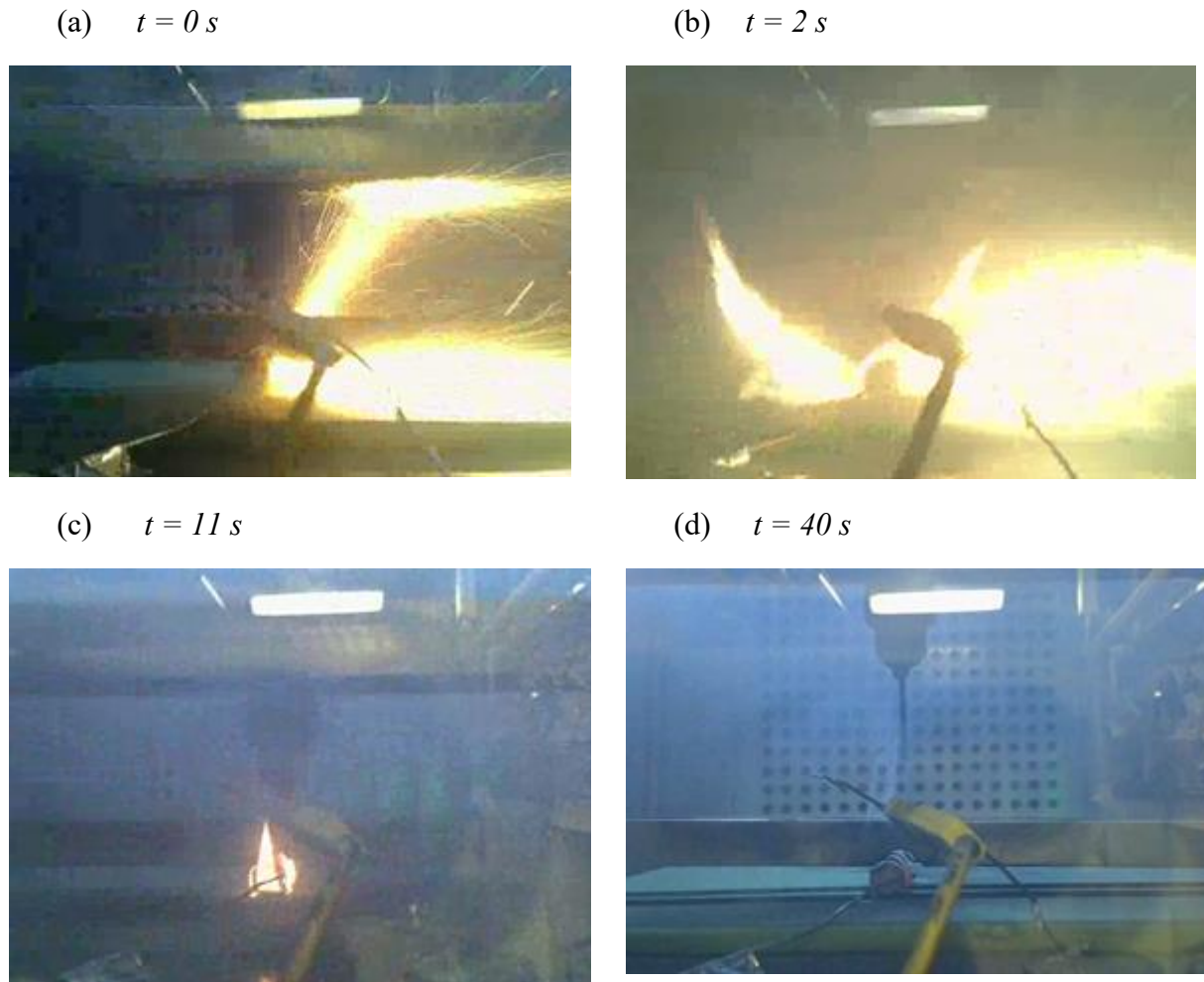


Figure 31: Sequence of NP-induced TR of the Efest (LMO) 18650 cell at 100% SOC: (a) venting and flame ejection from the penetration site ($t = 0\text{ s}$), (b) and (c) continued combustion, (d) complete flame extinction ($t = 40\text{ s}$)

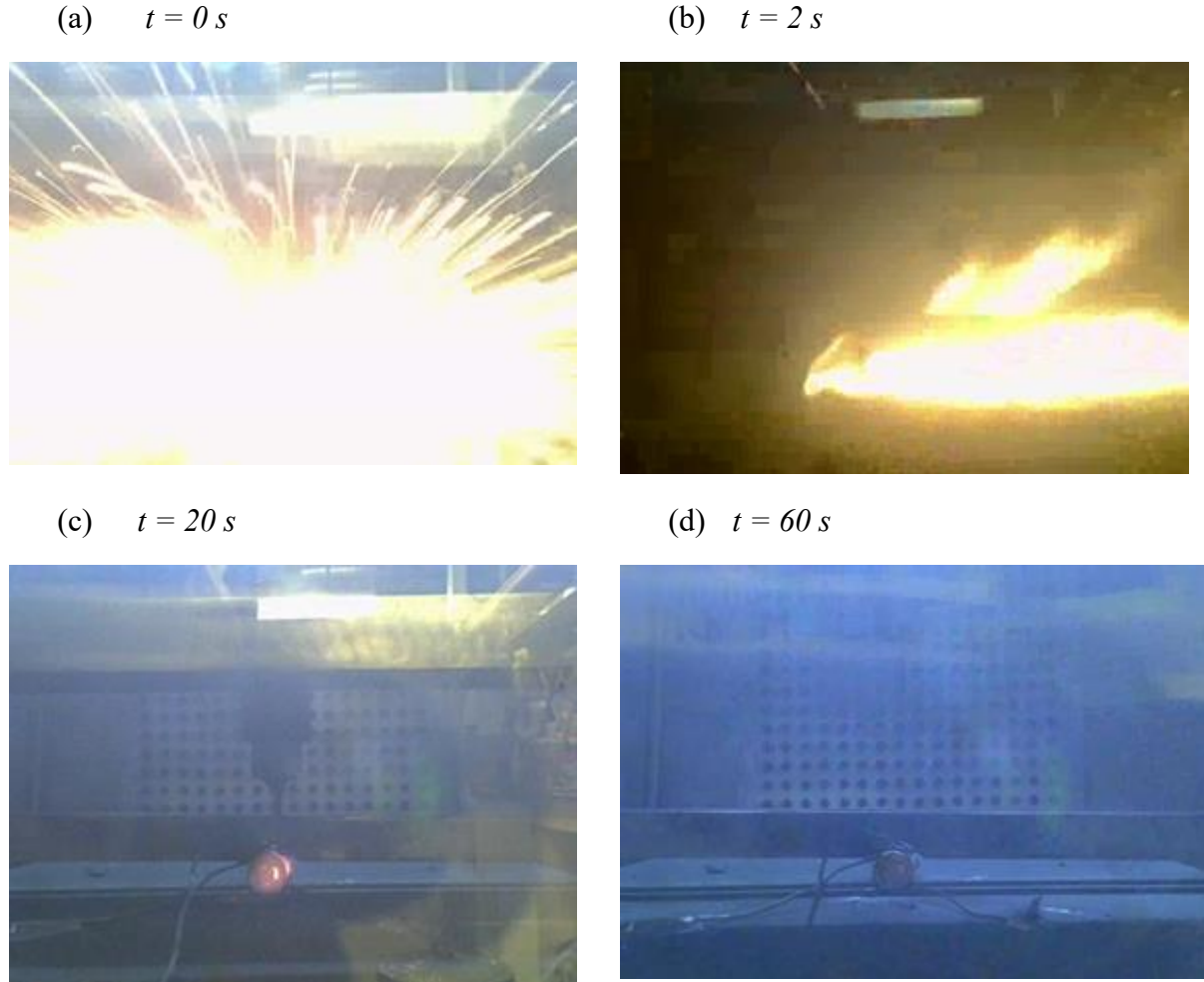


Figure 32: Sequence of NP-induced TR of the Samsung INR21700 (NCA) cell at 100% SOC: (a) venting and flame ejection from the penetration site ($t = 0\text{ s}$), (b) and (c) continued combustion, (d) complete flame extinction ($t = 60\text{ s}$)

Among the cylindrical cells, the Samsung INR21700 underwent the most visually severe TR, producing the most intense flames and the highest measured peak surface temperature ($\sim 800^{\circ}\text{C}$). In contrast, the Samsung INR18650 had the shortest combustion duration (17 s), while the Panasonic NCR18650 maintained flaming combustion for approximately one minute. These observations suggest that although immediate ignition is characteristic of cylindrical LIBs at high SOC, the subsequent progression of TR is strongly influenced by cell chemistry, capacity, and design.

A distinctly different ignition behaviour was observed for the Kokam 40 Ah pouch cell, as shown in **Figure 33**. Unlike the cylindrical cells, NP initially produced only localized heating and sustained smoke emission, while the cell voltage decreased only slightly, indicating that a complete internal short circuit had not yet developed. Delayed ignition occurred several minutes later following removal of the nail, after which the cell entered sustained TR with combustion lasting approximately 13 minutes. This behaviour illustrates that the absence of immediate ignition following NP does not necessarily imply that the cell has reached a safe condition. Instead, thermal and electrochemical reactions may continue to develop within the cell, resulting in ignition well after the initial abuse event.

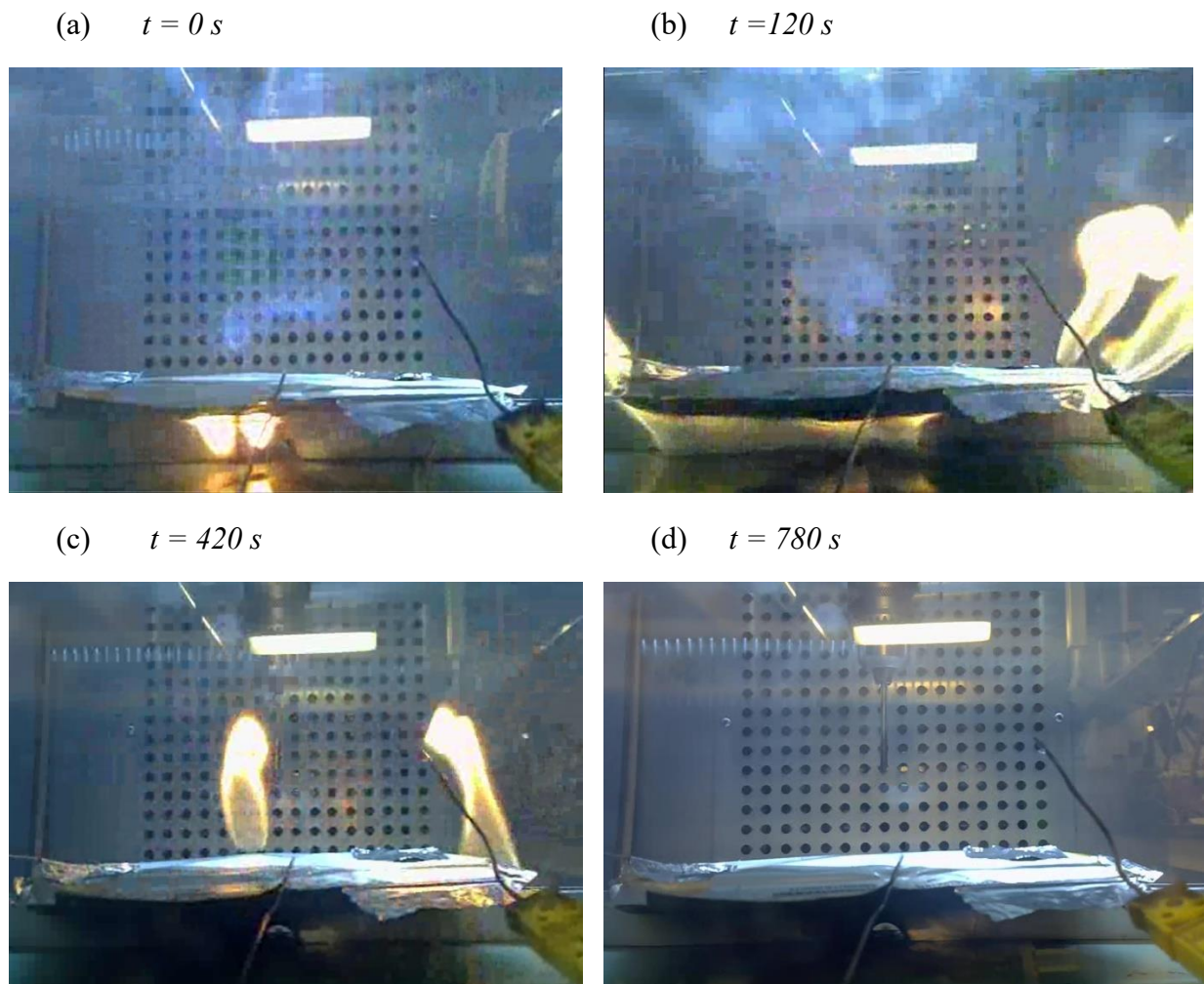


Figure 33: Sequence of NP-induced TR of the Kokam Pouch cell at 100% SOC: (a) Cell ignition approx. 2 minutes post nail retraction ($t = 0$ s), (b), (c) continued combustion, (d) complete flame extinction ($t = 780$ s)

The influence of SOC on ignition behaviour was consistently observed across the LG-HG2, Panasonic NCR18650, Efest IMR18650, and Samsung INR21700 cells, all of which were investigated over a range of SOC. At high SOC, the energy available within the cell was sufficient to rapidly initiate self-sustaining exothermic reactions following NP, resulting in immediate TR accompanied by sustained flaming combustion. As SOC decreased, the severity of the event progressively diminished, eventually transitioning from sustained combustion to smoke generation alone. The SOC threshold for TR varied between chemistries, with the Panasonic NCR18650 exhibiting TR down to approximately 90% SOC, whereas the Efest IMR18650, Samsung INR21700, and LG-HG2 cells continued to undergo TR at approximately 70–77% SOC as highlighted in **Table 7**. Below these thresholds, NP generally produced only smoke or brief ejecta without sustained flaming combustion. These observations suggest that although the critical SOC for TR initiation depends on battery chemistry and design, increasing SOC consistently increases the likelihood and severity of NP-induced TR.

5.3.2 Venting Behaviour

The location from which combustion products were released during NP-induced TR varied considerably among the studied cells and was found to depend mainly on cell design rather than chemistry alone. Two distinct venting behaviours were observed: venting through the cell rupture plate and venting directly from the penetration site.

The Samsung INR18650 and Samsung INR21700 cells consistently expelled high-temperature ejecta through the rupture plate located at the positive terminal of the cell. In both cases, the initial release of gases and PM occurred through the safety vent before transitioning into sustained flaming combustion. This behaviour implies that the internal pressure generated during TR was preferentially relieved through the engineered pressure-relief mechanism incorporated into the cell design.

In contrast, the LG-HG2, Panasonic NCR18650, and Efest IMR18650 cells primarily vented through the penetration site. Following NP, flames and ejecta emerged directly from the nail opening rather than from the rupture plate, suggesting that the penetration channel provided the path of least resistance for the release of gases and molten materials. The Kokam pouch cell exhibited a similar venting location following delayed ignition, with combustion originating from

the damaged region surrounding the penetration site. These observations indicate that the location of venting is not governed by the cell chemistry alone, as cells employing similar NMC chemistries showcased different venting behaviours.

The observed differences are likely associated with variations in cell construction, including the design of the pressure-relief vent, internal gas flow pathways, and the mechanical response of the cell casing during NP. Although the precise mechanisms governing vent location were beyond the scope of the present work, the results demonstrate that battery design plays a significant role in determining how gases and combustion products are released during TR.

From a safety perspective, the venting location has important implications for the direction of flame propagation, heat transfer to surrounding components, and the dispersion of PM generated during TR. Consequently, venting behaviour should be considered alongside cell chemistry and capacity when assessing the hazards associated with mechanical abuse of commercial LIBs.

5.3.3 Influence of Cell Chemistry and Form Factor

The results presented in sections 5.3.1 and 5.3.2 demonstrate that both cell chemistry and physical design influence the progression of NP-induced TR. Although all investigated cells underwent internal short-circuit formation following penetration, noticeable differences were observed in combustion intensity, venting behaviour, and overall failure progression.

Among the cylindrical cells, the three NMC cells had generally similar ignition characteristics, with immediate TR occurring at high SOC. However, increasing cell capacity resulted in more severe thermal events. The Samsung INR21700 cell produced the highest measured surface temperature and the most intense flaming combustion, whereas the Samsung INR18650 and LG-HG2 cells experienced comparatively less severe events. This trend is consistent with the greater electrochemical energy stored within the larger-capacity cell.

The Panasonic NCR18650B (NCA) cell displayed prolonged flaming combustion compared with the cylindrical NMC cells despite having a lower peak temperature than the Samsung INR21700. In contrast, the Efest IMR18650 (LMO) cell displayed combustion behaviour comparable to the Panasonic cell but maintained TR at lower SOC. These observations suggest that although chemistry influences the progression and severity of TR, the relationship is not governed by

chemistry alone. Cell construction, electrode design, and energy content also contribute significantly to the observed differences.

The pouch cell on the other hand, experienced delayed ignition after an extended period of smoke generation following penetration. Unlike cylindrical cells, which rely on rigid metallic casings and pressure-relief mechanisms, the flexible pouch cell casing allows deformation and localized damage which could alter the development of internal short circuits and gas release pathways. **Figure 33** is a clear example of this mechanism where the ignition occurred at the bottom of the pouch cell after minutes of smoke generation, indicating how the progression of TR in these cells may differ substantially from that observed in cylindrical formats.

Altogether, the results confirm that NP-induced TR cannot be attributed solely to battery chemistry. The interaction between chemistry, cell capacity, and structural design controls the initiation and progression of TR. These findings emphasize the importance of considering the complete cell architecture when evaluating battery safety under mechanical abuse.

5.3.4 Summary

A qualitative comparison of the investigated LIBs showed that NP-induced TR follows a broadly similar sequence consisting of venting, ignition, combustion, and eventual extinction. However, the progression of these stages varied considerably depending on the cell chemistry, capacity, form factor, and SOC. Immediate TR was the predominant response among cylindrical cells tested at high SOC, whereas the Kokam pouch cell underwent delayed ignition several minutes after penetration, highlighting the influence of cell construction on failure progression.

The location of venting also differed between the investigated cells. The Samsung INR18650 and Samsung INR21700 cells released flames and ejecta through the rupture plate, whereas the LG-HG2, Panasonic NCR18650B, Efest IMR18650, and Kokam pouch cell vented primarily from the penetration site. These differences indicate that venting behaviour is governed not only by battery chemistry but also by the design of the cell and its pressure-relief features.

Among the cylindrical cells, increasing SOC consistently produced more severe TR, while reducing SOC progressively suppressed combustion until only smoke generation remained. Nevertheless, the SOC threshold required to sustain TR differed between cell types, demonstrating that the influence of SOC is closely linked to battery chemistry and design. Overall, the comparison

presented in this chapter highlights that the response of LIBs to NP cannot be generalized across different battery technologies, emphasizing the need to consider the combined effects of chemistry, cell architecture, and operating conditions when assessing battery safety under mechanical abuse.

Chapter 6 Particulate Characterization of Thermal Runaway Ejecta from LG-HG2 Cells

6.1 Experimental Methodology

6.1.1 Sample Preparation

NP experiments were conducted on a commercial LG-HG2 18650 Li-ion cell at 100% SOC. During TR, the solid ejecta was collected onto a clean glass substrate positioned directly above the cell venting region, as shown in **Figure 34 (a)**. This configuration ensured interception of high-velocity Particulate Matter (PM) emitted during the venting and subsequent combustion phases.

Following the experiment, two separate sample preparation approaches were employed depending on the analytical objective. For XRD analysis, the collected particle was scraped from the glass substrate and mechanically ground using a mortar and pestle for approximately 10 minutes to obtain a fine and homogeneous powder, as shown in **Figure 34 (b)**. The grinding process improved sample uniformity and dispersion for bulk phase analysis.

For detailed SEM-EDX characterization and particle size distribution (PSD) analysis, a separate portion of the collected particle was preserved in its native, unground state in order to maintain the original particle morphology, agglomeration structure, and size distribution generated during TR. Preserving the native particulate structure enabled subsequent morphology classification and quantitative PSD analysis of the emitted particles.

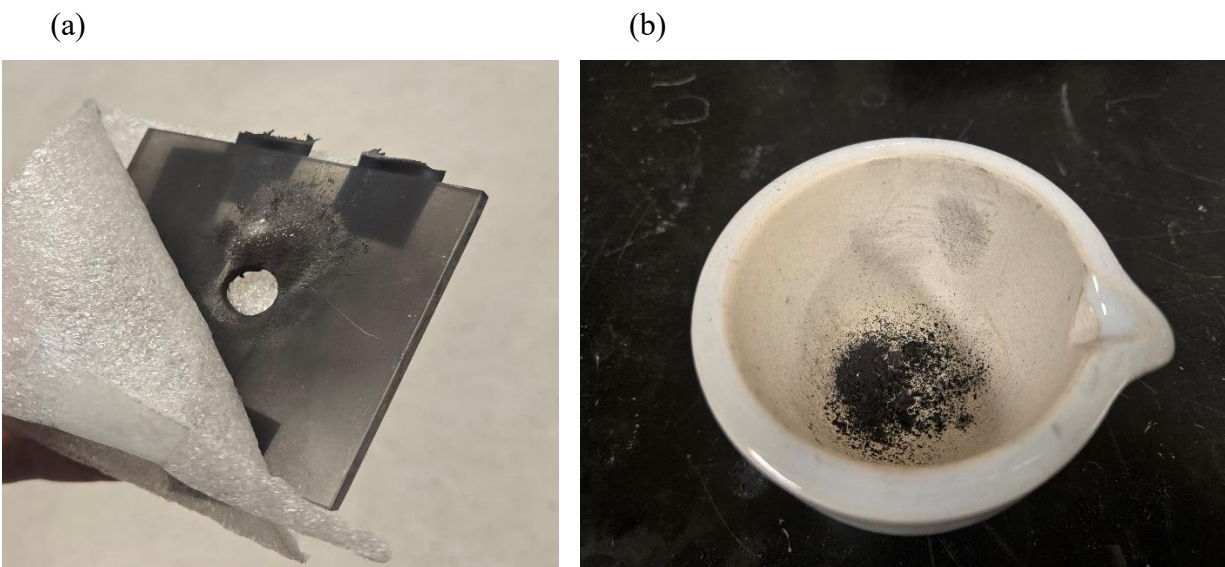


Figure 34: Particle collection and sample preparation procedure for post-TR analysis. (a) Deposit of solid ejecta on a glass substrate positioned above the cell to capture particulate matter emitted during venting and combustion. (b) Mechanically ground particles using a mortar and pestle prior to XRD analysis to obtain a fine and homogeneous powder

6.1.2 Scanning Electron Microscopy and EDX Methodology

Morphological and elemental characterization of the TR particles was performed using SEM coupled with EDX. The imaging was conducted using a Zeiss FESEM 1530 field-emission scanning electron microscope.

All particle samples were mounted on conductive carbon tape affixed to aluminum stubs and subsequently sputter-coated with a thin layer of gold (Au) to improve surface conductivity and minimize charging during analysis. SEM imaging was performed at an accelerating voltage (EHT) of 10 kV. EDX analysis was conducted on multiple regions of each sample to account for spatial variability in composition. Elemental mapping and compositional analysis were performed for C, O, F, Al, Si, Mn, Mg, Cu, Ni, Co, P, and S.

Due to the use of conductive carbon tape for sample mounting, the detected carbon signal contains contributions from both the sample and the substrate. Consequently, carbon maps were interpreted qualitatively, while greater emphasis was placed on the spatial distribution of the remaining detected elements when assessing particle composition.

6.1.3 X-ray Diffraction (XRD) Analysis

Phase characterization of the TR particle was conducted using X-ray diffraction (XRD). Measurements were performed using a Rigaku MiniFlex II diffractometer equipped with a Cu K α radiation source ($\lambda = 1.54059 \text{ \AA}$) and a scintillation detector.

The mechanically ground particles described in Section 6.1.1 was mounted onto the sample holder and gently pressed to obtain a flat and uniform surface suitable for diffraction analysis, as shown in **Figure 35 (a) and (b)**.

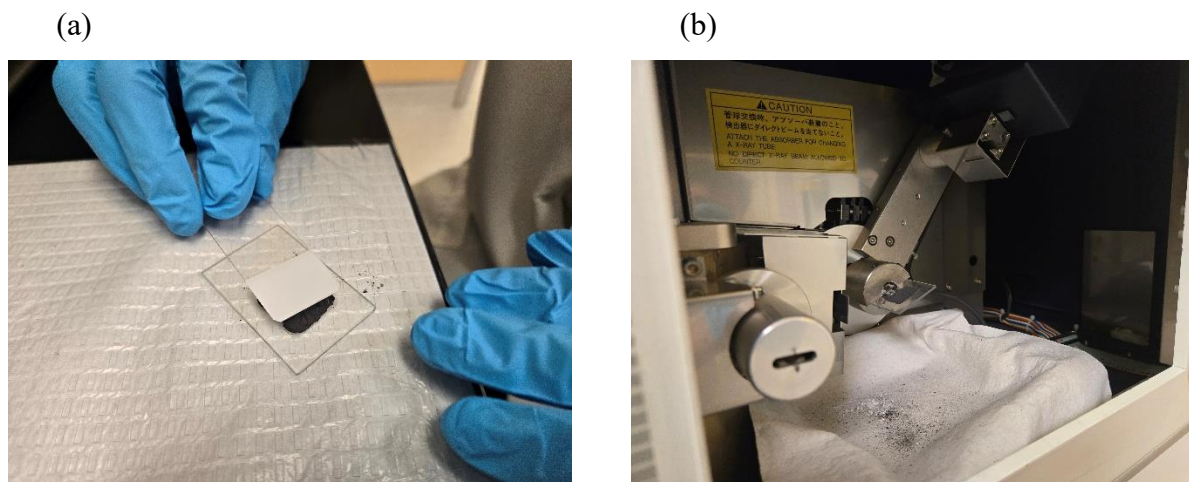


Figure 35: (a) Ground particle sample mounted on the XRD sample holder, (b) sample on the XRD machine prior to diffraction analysis

Diffraction data were collected over a 2θ range of 3° to 90° with a step size of 0.02° . These parameters were selected to capture diffraction peaks corresponding to crystalline phases commonly associated with LIB TR products. Intensity data were recorded as a function of diffraction angle (2θ), and the resulting diffraction patterns were analyzed for phase identification of crystalline species present in the TR particles.

6.2 Results

The particulate matter (PM) generated during TR was characterized using SEM-EDX and XRD to investigate particle morphology, size distribution, elemental composition, and crystalline phase composition. The results revealed a heterogeneous particulate population consisting of carbonaceous particles, metallic fragments, and metal-containing compounds originating from multiple particulate formation pathways during TR.

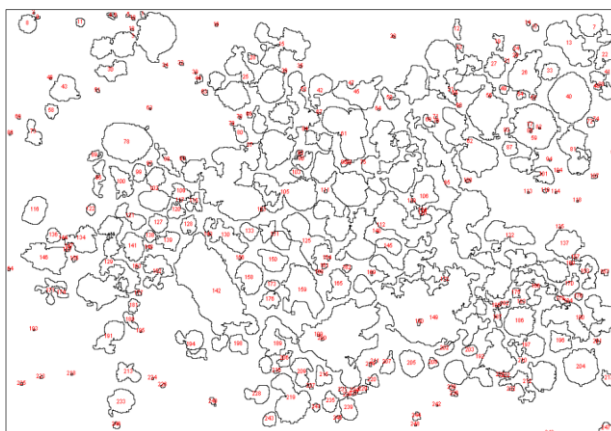
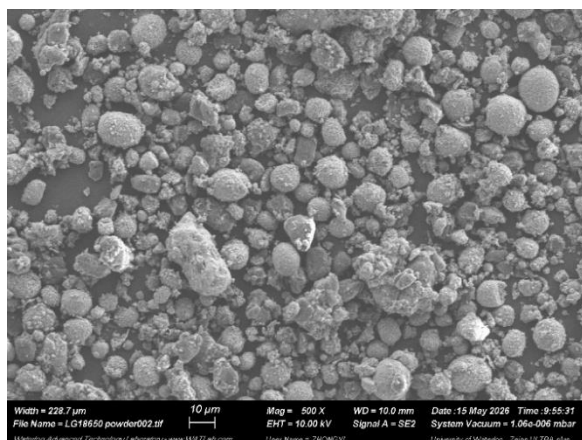
6.2.1 SEM-EDX: Results from Detailed Characterization

The unground TR particle samples observed on the carbon tape substrate from SEM imaging are presented on the left-hand side of **Figure 36 (a)–(c)**. The sample surface appears to be extensively covered with particulates exhibiting a wide range of particle sizes and morphologies, indicating the heterogeneous nature of the TR ejecta. Closer examination of the micrographs reveals several distinct particle classes, including predominantly spherical particles with rough or porous surfaces, irregular fractured fragments with no well-defined geometry, submicron-scale particles deposited either individually or in small clusters, elongated flaky structures, and occasional larger agglomerates formed through particle accumulation.

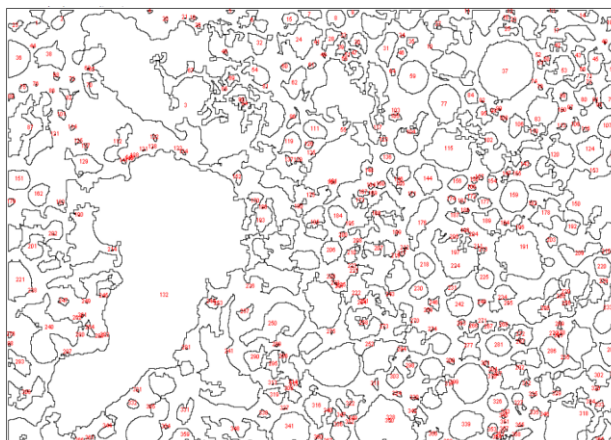
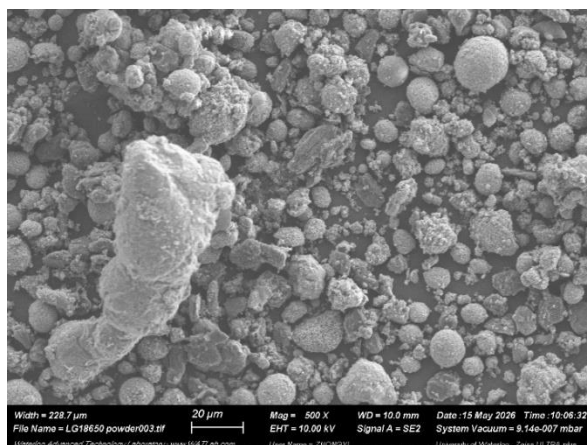
The coexistence of spherical particles, irregular fragments, agglomerates, and flake-like structures is consistent with previous studies of TR-generated PM. Similar spherical and fragmented particles have been reported by Chen et al. and Barone et al. for NMC cells, while Grossetête et al. observed elongated flake-like structures associated with larger particulate deposits [81], [84], [88]. The broad range of particle morphologies observed in the present study further supports the heterogeneous and multi-scale nature of particulate emissions generated during TR.

To quantitatively characterize the observed particle population, image segmentation was performed using the Trainable Weka Segmentation plugin in Fiji, which employs the FastRandomForest machine learning algorithm to separate PM from the background substrate. Prior to segmentation, manual thresholding was applied to improve particle-background contrast and minimize false particle detection, as shown on the right-hand side of **Figure 36 (a)–(c)**.

(a) Region #1



(b) Region #2



(c) Region #3

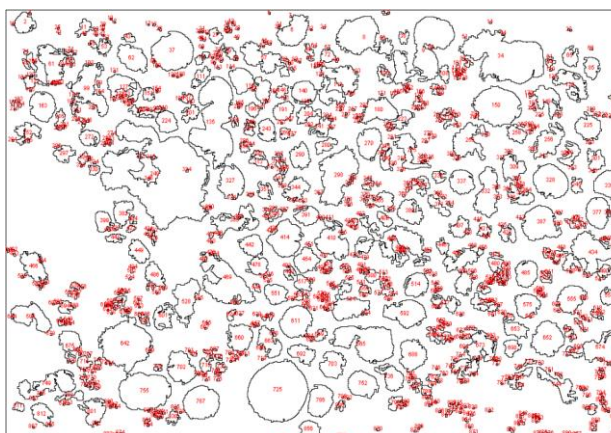
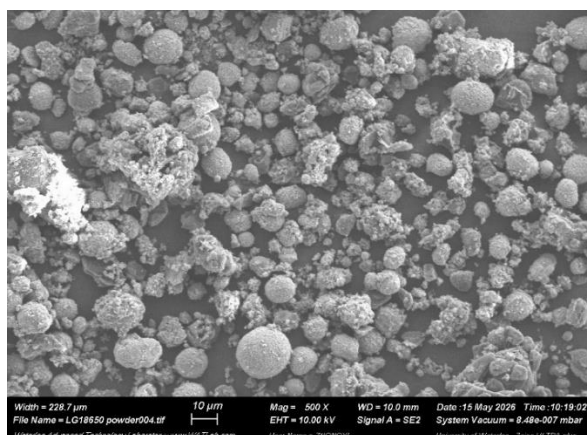


Figure 36: SEM micrographs of unground TR particles collected following NP-induced TR of an LG-HG2 cell. Images (a), (b), and (c) show the diverse particle morphologies and size distributions present within different regions of the ejecta

Following image segmentation, the projected area of each detected particle was measured and converted into an equivalent circular diameter (ECD) using **Equation 2**. The resulting ECD values were used to construct both a normalized particle size distribution (PSD) and a cumulative particle size distribution in order to characterize the size distribution of particulates emitted during TR. The normalized PSD provides the relative frequency of particles within specific size intervals, while the cumulative PSD illustrates the proportion of particles below a given diameter and enables determination of characteristic particle diameters (D10, D50, and D90). The resulting distributions are presented in **Figure 37** and **Figure 38**.

$$ECD = 2 \cdot \sqrt{\left(\frac{A}{\pi}\right)} \quad (2)$$

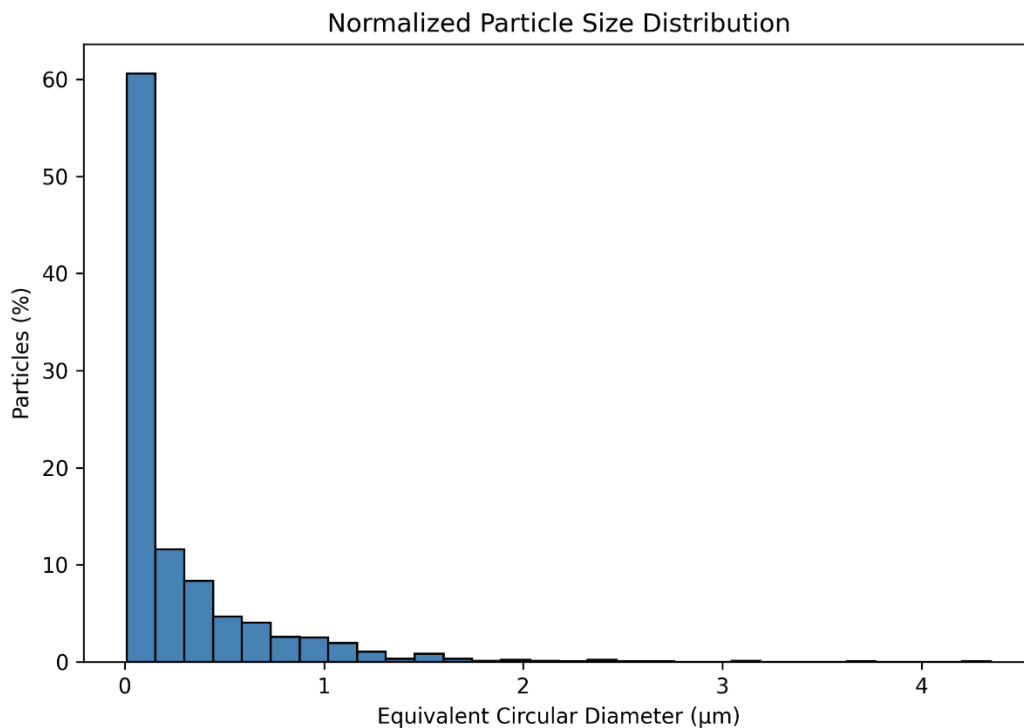


Figure 37: Normalized particle size distribution of TR ejecta based on the equivalent circular diameter (ECD) obtained from SEM image analysis. The distribution is strongly skewed toward smaller particle sizes, indicating that the particulate ejecta is predominantly composed of sub-micron particles

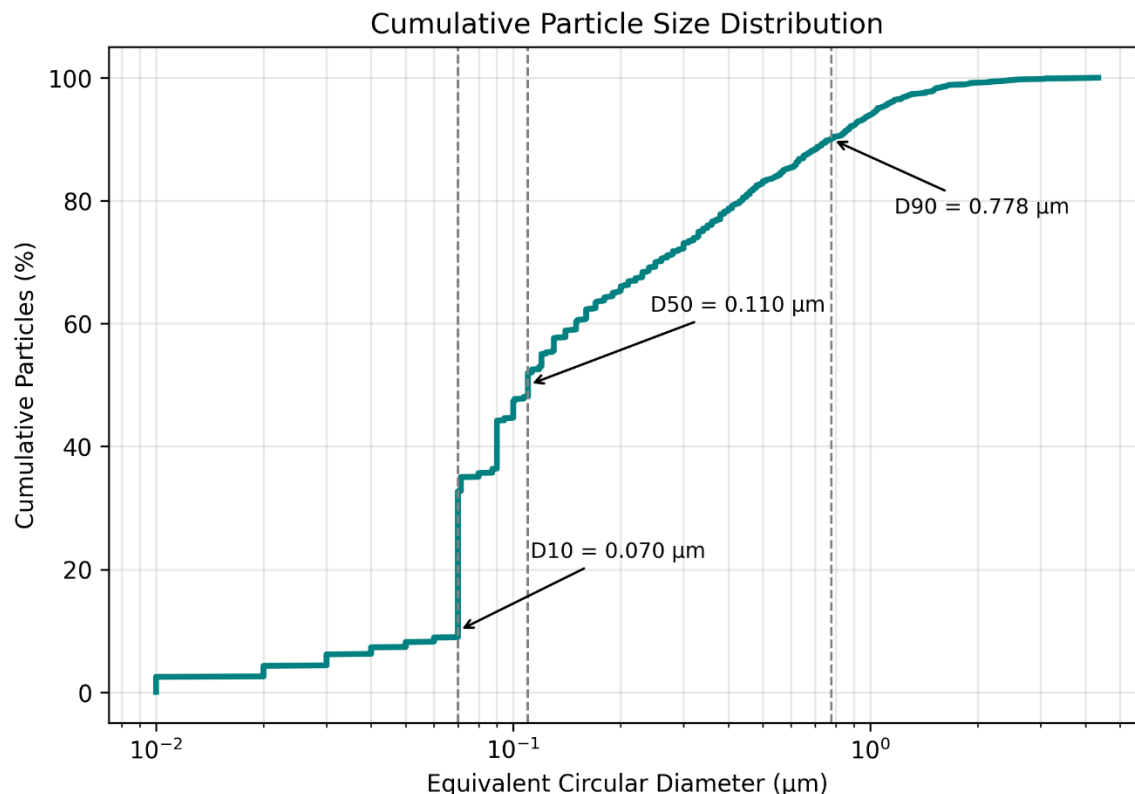


Figure 38: Cumulative particle size distribution of TR ejecta based on equivalent circular diameter (ECD) derived from SEM image analysis. The characteristic particle diameters corresponding to the 10th, 50th, and 90th percentiles of the distribution (D10, D50, and D90) are shown

The normalized PSD and cumulative PSD indicate that the emitted particulate was predominantly composed of submicron particles. The cumulative distribution yielded D10, D50, and D90 values of 0.070 μm, 0.110 μm, and 0.778 μm, respectively, indicating that 10%, 50%, and 90% of the detected particles possessed equivalent circular diameters below these values. The relatively small D50 value suggests that the particle population was dominated by fine PM, with half of all detected particles exhibiting diameters below 0.110 μm.

The PSD exhibits a strongly right-skewed distribution, characterized by a large population of small particles and a limited number of larger agglomerates extending the upper tail of the distribution. This behaviour is consistent with particle formation during TR, where rapid decomposition of

electrode and electrolyte materials generates a substantial number of fine particles while simultaneous coagulation and agglomeration processes produce a smaller population of larger structures. Although several large agglomerates were identified within the analysed samples, their low abundance relative to the total particle population had only a limited influence on the overall size distribution, which remained dominated by submicron particles.

The predominance of submicron particles suggests that a substantial fraction of the emitted PM may remain suspended for extended periods following cell failure, increasing the potential for transport away from the source region. These results therefore suggest that TR emissions from the investigated cell chemistry consist primarily of fine PM, accompanied by a comparatively small fraction of larger agglomerated debris.

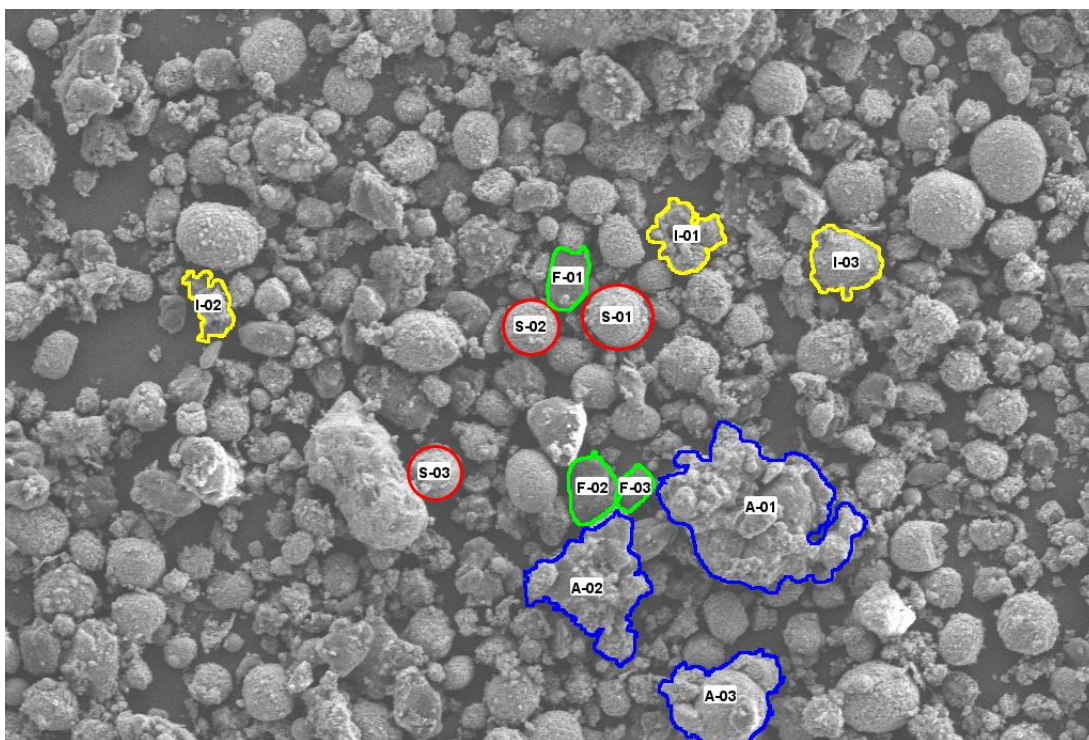
While the PSD analysis provides quantitative information regarding particle size, it does not distinguish between the various particle morphologies observed in the SEM micrographs. To further characterize the heterogeneous particulate population, particles identified from the segmented images were manually classified into four morphology categories: spherical, irregular, agglomerated, and flake-like particles. This classification provides a more detailed assessment of the physical characteristics of TR-generated PM and supports interpretation of the mechanisms responsible for particle formation during TR.

Classification was performed based on projected particle geometry and surface appearance observed in the SEM micrographs. Spherical particles were identified by their near-circular morphology and smooth boundaries, while irregular particles had non-uniform geometries lacking distinct structural symmetry. Agglomerated particles consisted of clustered or chain-like assemblies of smaller primary particles, indicative of particle coagulation or aggregation behaviour. Flake-like particles were characterized by thin, plate-like morphologies with relatively large projected surface areas and irregular planar structures.

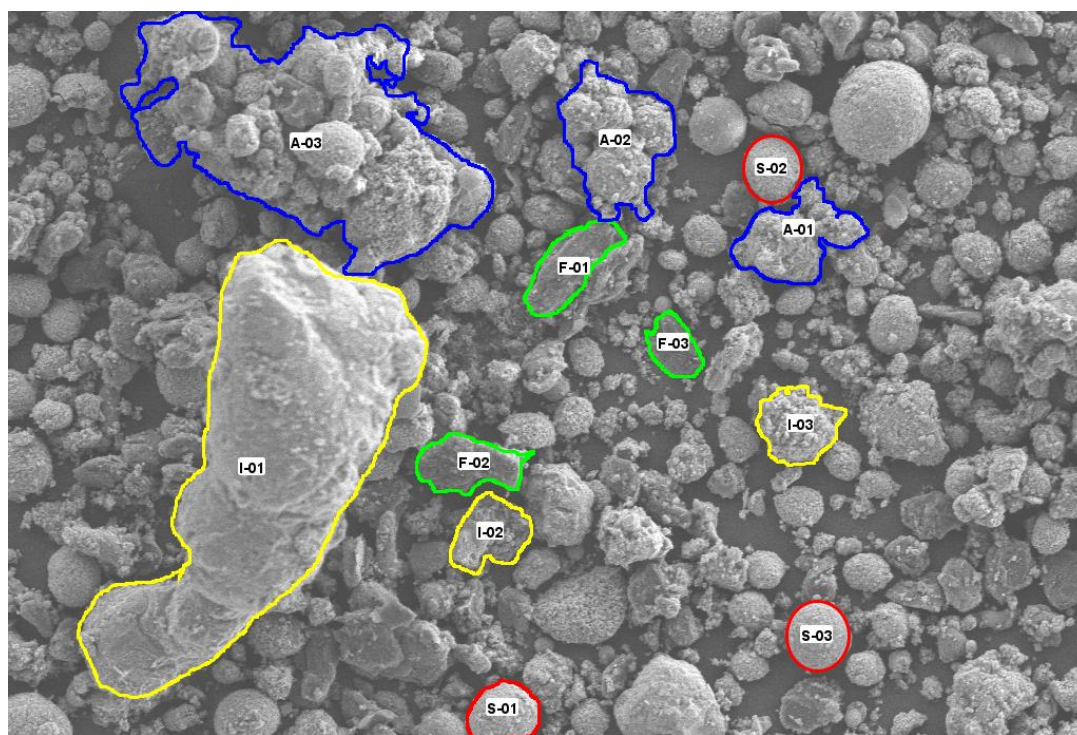
Representative particles from each morphology category were annotated directly on the SEM images using colour-coded overlays to facilitate qualitative comparison between particle classes, as shown in **Figure 39**. For each morphology category, three representative particles were selected and assessed using EDX to identify the dominant elemental signatures associated with that particle class. The resulting classification highlights the morphological diversity present within the emitted PM. The coexistence of spherical particles, agglomerates, flakes, and irregular fragments suggests

that multiple particulate formation pathways were active during TR, including condensation, agglomeration of primary particles, and mechanical fragmentation of electrode materials under elevated temperature and pressure conditions.

(a) Region #1



(b) Region #2



(c) Region #3

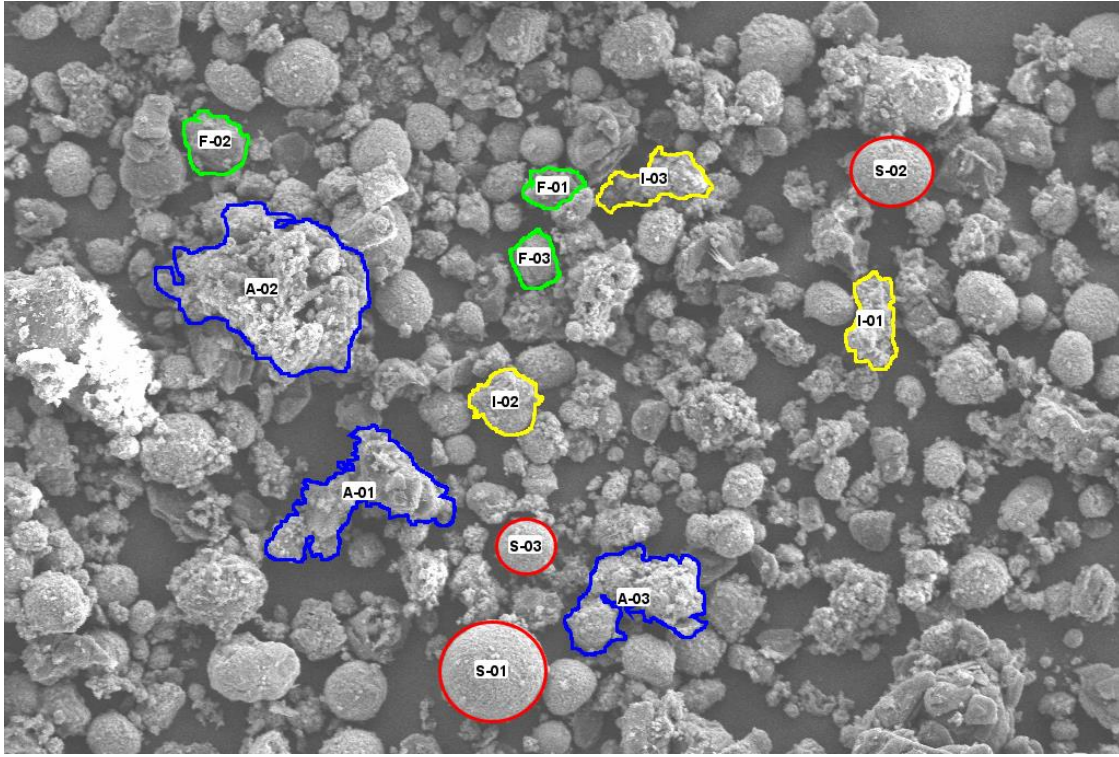


Figure 39: (a), (b), (c) Representative SEM micrographs showing manually classified particle morphologies observed in TR-generated particles, including spherical, irregular, agglomerated, and flake-like particles

Table 8: Summary of particle morphologies observed in the TR ejecta, together with representative equivalent circular diameters (ECDs), dominant elemental composition, and proposed particle origins

Morphology	Representative Size Range (ECD, μm)	Representative Dominant Elements	Interpretation
Spherical	0.70 - 2.133	Nickel, Cobalt	The spherical morphology suggests melting and subsequent solidification of the NMC electrode material during the high temperature TR. The high T_s and T_{ej}

			values recorded at high SOCs, together with the observed high velocity flame ejecta, indicate that the molten cathode material was carried along with the ejecta before it rapidly cooled to form spherical particles.
Agglomerated	Variable	Aluminum, Carbon	Agglomerated particles containing both carbonaceous material and Al-containing species, suggest particle coagulation and incorporation of fragmented cell components during the prolonged venting phase where particle collisions may have likely occurred.
Flake-like	0.56- 1.20	Carbon	Carbon-rich flaky structures are likely derived from fragmented carbonaceous battery materials including graphite or conductive carbon additives, together with residues formed from electrolyte decomposition. Their morphology agrees with the extensive particle material observed on the current collector surfaces following TR as discussed in Chapter 6.
Irregular	Variable	Aluminum, Fluorine, Phosphorous	The irregular morphology and heterogenous elemental composition suggest fragmentation of battery components during TR. This interpretation is further supported by observations from the penetration region of the disassembled cell, presented later in Chapter 6, suggesting that these particles were formed

			by the severe mechanical disruption occurring at the penetration region, together with deposition of electrolyte (LiPF ₆) decomposition products.
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The morphology–composition relationships summarized in **Table 8** show that distinct particle morphologies were associated with different elemental signatures. Spherical particles were primarily enriched in Ni and Co, suggesting an origin associated with cathode-derived materials ejected during TR. Agglomerated particles contained both Al and C, indicating the coexistence of carbonaceous material and Al-containing species within particle clusters. Flake-like particles were predominantly C-rich, while irregular particles showcased a more complex composition containing Al, F, and P, suggesting contributions from multiple battery components and electrolyte decomposition products.

The observed variation in both morphology and elemental composition supports the presence of multiple particulate formation pathways during TR. The coexistence of Ni- and Co-rich spherical particles, carbon-rich flaky structures, Al-containing agglomerates, and chemically heterogeneous irregular fragments suggests that particle generation resulted from a combination of cathode material ejection, particle agglomeration, condensation of decomposition products, and mechanical fragmentation of internal cell components.

To investigate the elemental composition associated with the identified particle morphologies, EDX elemental mapping was performed on the three representative SEM regions used for morphology analysis. Carbon, oxygen, nickel, and aluminum were selected for presentation in the main text due to their relevance to the carbonaceous particle matrix and key LIB components. The corresponding elemental maps are presented in **Figure 40-42**.

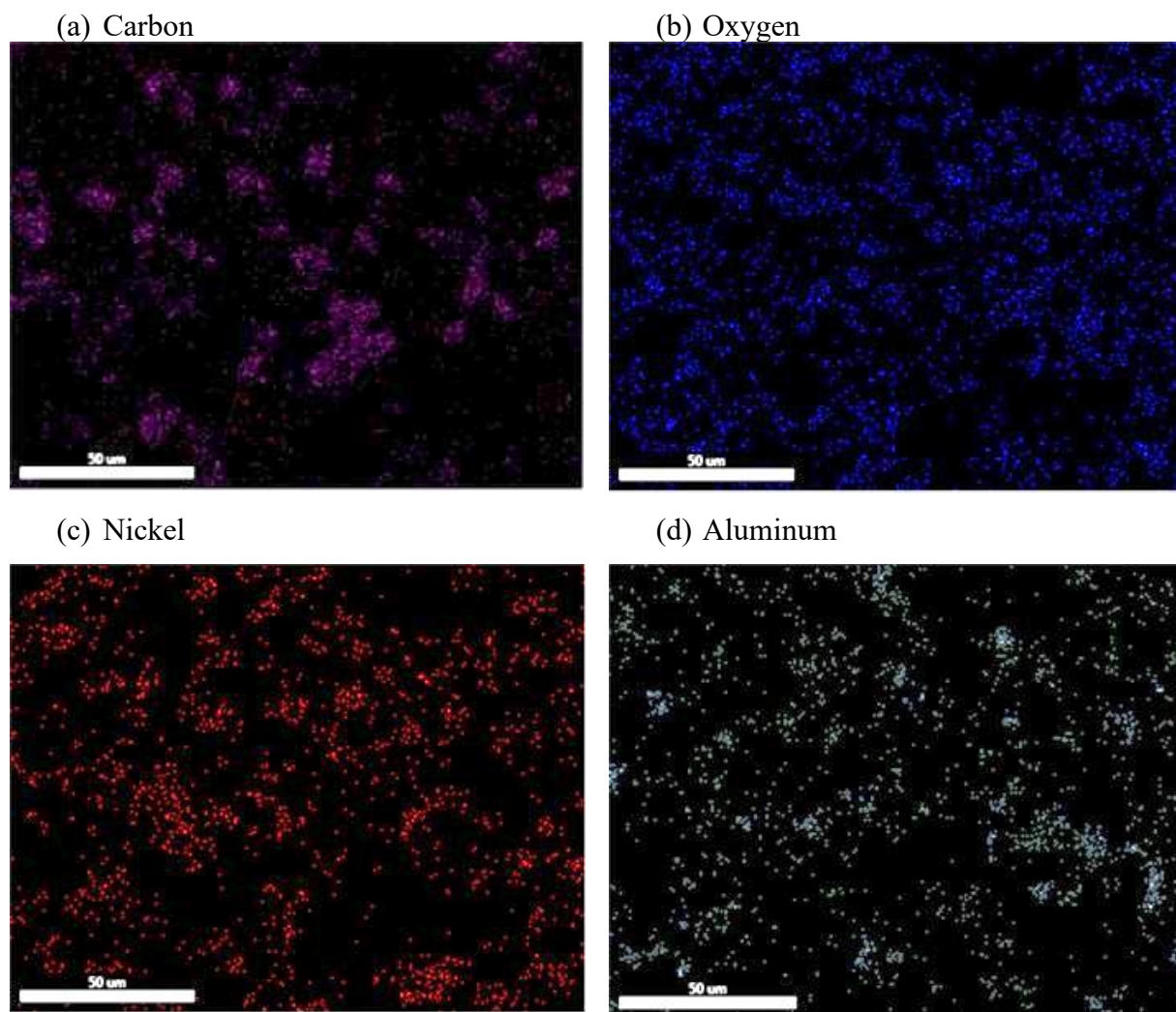


Figure 40: EDX elemental maps of (a) carbon (C), (b) oxygen (O), (c) nickel (Ni), and (d) aluminum (Al) for representative Region 1 of the unground TR particle sample collected from the LG-HG2 cell following NP-induced TR

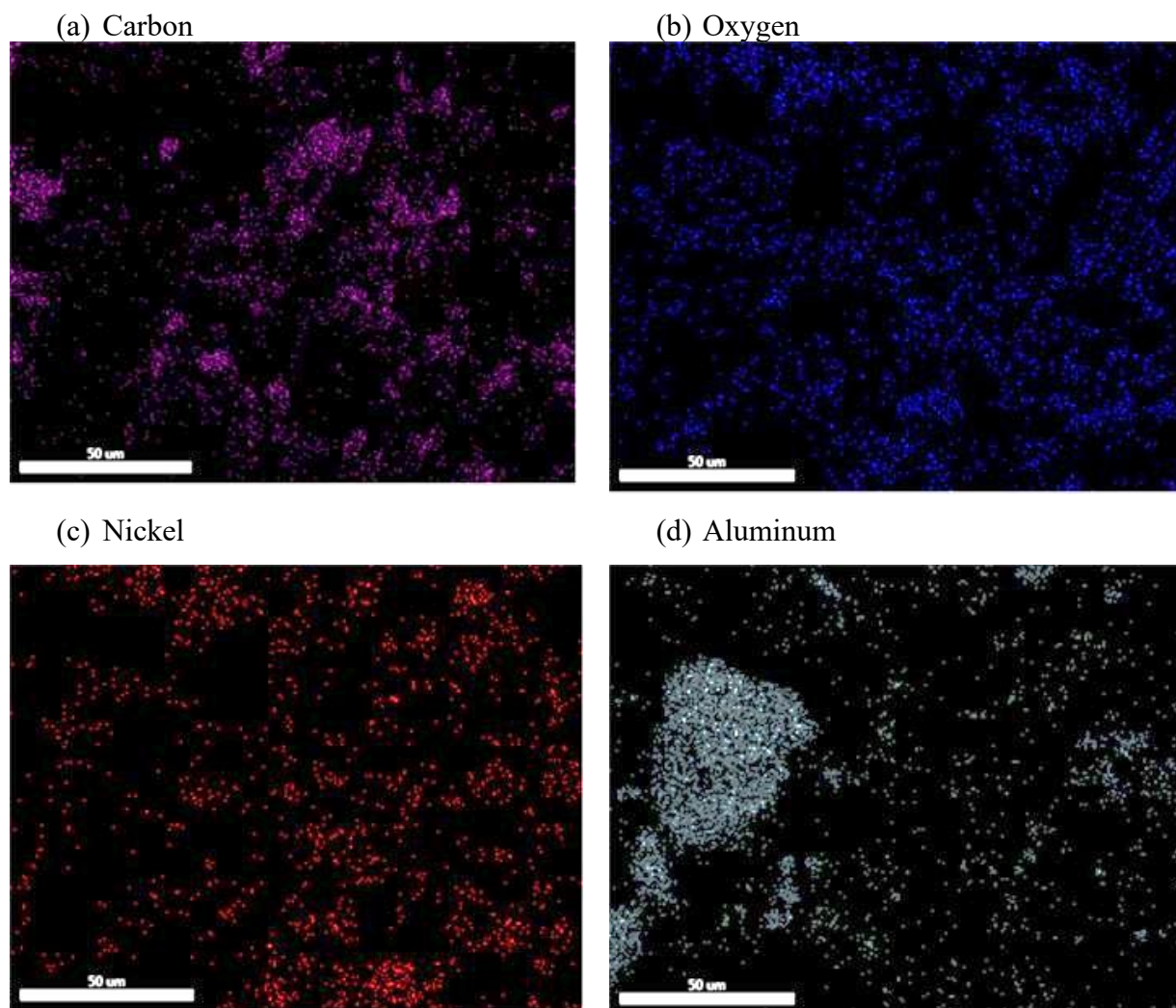


Figure 41: EDX elemental maps of (a) carbon (C), (b) oxygen (O), (c) nickel (Ni), and (d) aluminum (Al) for representative Region 2 of the unground TR particle sample collected from the LG-HG2 cell following NP-induced TR

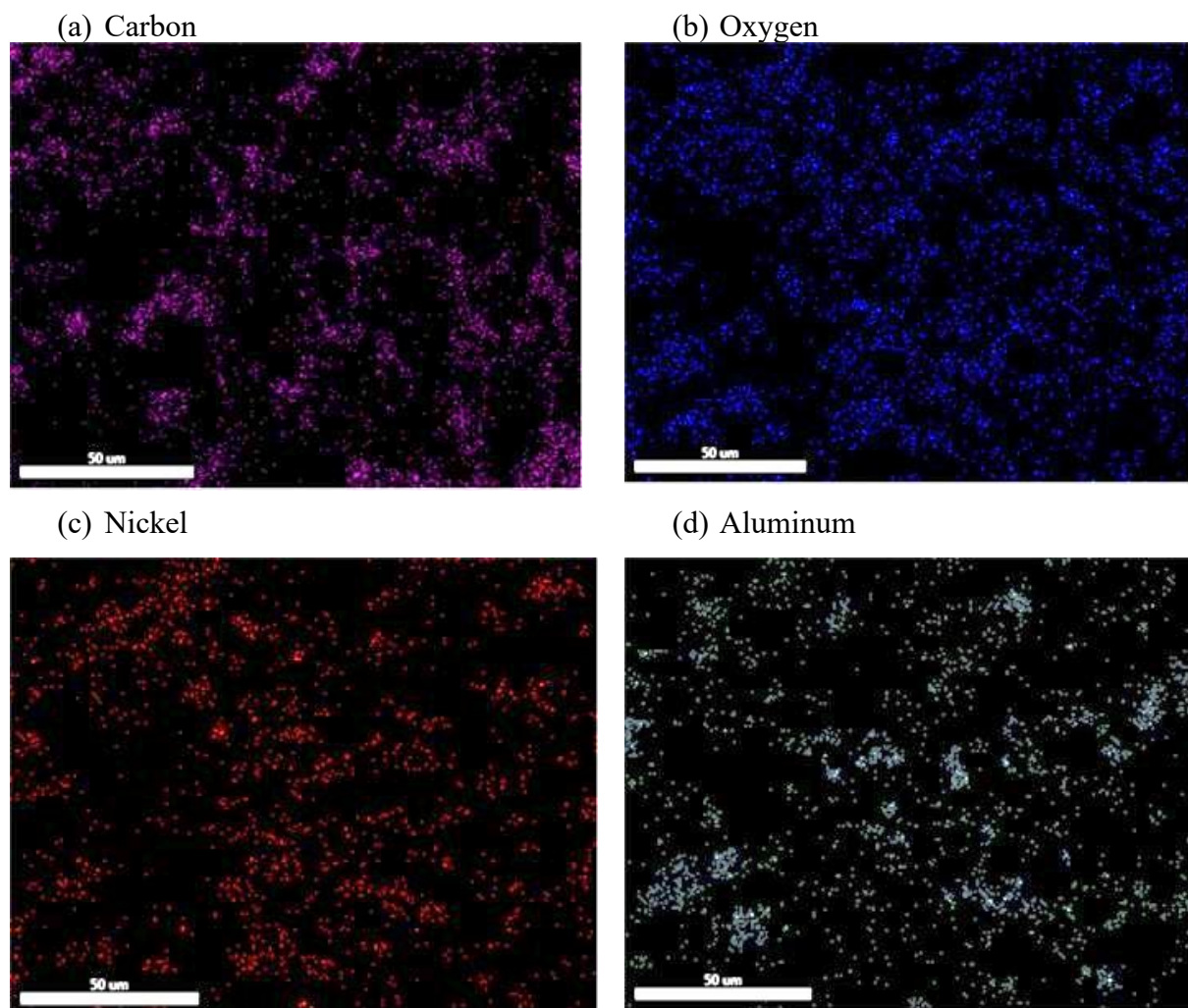


Figure 42: EDX elemental maps of (a) carbon (C), (b) oxygen (O), (c) nickel (Ni), and (d) aluminum (Al) for representative Region 3 of the unground TR particle sample collected from the LG-HG2 cell following NP-induced TR

Carbon was observed throughout the analysed regions and had the greatest spatial coverage among all mapped elements. Localized regions of elevated carbon intensity were associated with individual particles and particle agglomerates; however, some contribution from the carbon tape substrate is expected, particularly in areas of low particle density. Nevertheless, the widespread carbon distribution is consistent with the carbonaceous particles generated during TR.

Oxygen was similarly distributed across much of the sample surface and was frequently associated with particulate deposits. The presence of oxygen suggests the formation of oxygen-containing

species during the high-temperature TR process, including potential metal oxides and oxidized carbonaceous products.

Nickel and aluminum were primarily concentrated within discrete particles rather than being uniformly distributed throughout the sample. Nickel-rich particles were observed at several locations across all analysed regions, consistent with the presence of cathode-derived material originating from the NMC electrode. In contrast, aluminum was detected in more isolated regions, likely corresponding to fragments originating from the aluminum current collector or other aluminum-containing cell components.

Collectively, the elemental maps indicate that the emitted PM consists of a heterogeneous mixture of carbonaceous particles and metal-containing particles. The coexistence of C-rich deposits together with Ni- and Al-containing particulates suggests that both combustion-related processes and mechanical disruption of internal cell components contributed to particulate generation during TR.

6.2.2 SEM-EDX: Post Thermal Runaway Examination of Internal Cell Components

EDX analysis of the emitted PM revealed significant concentrations of Al-containing particles, whereas Cu-containing particles were detected only in trace amounts. Since both Al and Cu are major constituents of LIBs as current collector materials, this disparity prompted further investigation into the fate of these components during TR. To examine whether Cu-containing materials remained within the cell following failure, a representative LG-HG2 cell was disassembled after NP-induced TR, as shown in **Figure 43a**. The exposed internal components were subsequently examined using SEM-EDX (**Figure 43b**).

Visual inspection of the disassembled cell revealed that substantial portions of the Cu current collector remained intact, largely preserving the original jelly-roll structure. In contrast, the separator, electrode coatings, and Al current collector had undergone extensive degradation, leaving carbonaceous deposits adhered to the Cu surface. The preferential retention of the Cu current collector is consistent with the large difference in melting temperatures of the two current collectors. Aluminum melts at approximately 660 °C, whereas Cu remains solid until temperatures exceeding 1000 °C. The polymer separator and electrode binder materials decompose at considerably lower temperatures, explaining the extensive degradation observed following TR.

To further investigate the distribution of reaction products within the failed cell, residue samples were collected from three locations along the Cu current collector: the top, penetration (middle), and bottom regions of the cell cross-section. These locations were selected to determine whether the chemical composition of the post-TR residue varied spatially within the cell. The penetration region corresponds to the location of the internal short circuit and is therefore expected to experience the most severe thermal and electrochemical reactions. The top region is located adjacent to the rupture plate, where vent gases and PM are released during TR, while the bottom region is furthest from both the penetration site and rupture plate and was expected to experience the least severe local effects. Comparing these three locations provides insight into how decomposition products are distributed within the cell following NP-induced TR.

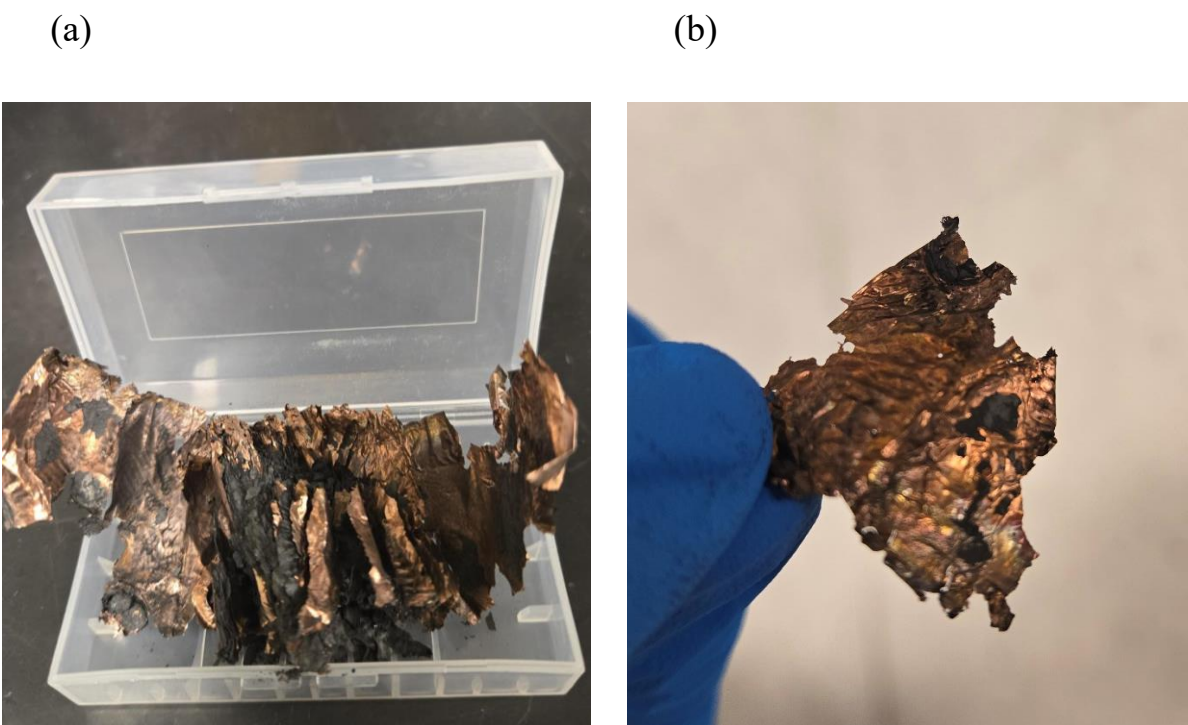


Figure 43: (a) Disassembled LG-HG2 cell following NP-induced TR showing the exposed internal components. (b) Representative SEM sample prepared from the retained Cu current collector for post-TR residue analysis

6.2.3 SEM-EDX: Spatial Variation of Residue Composition post Thermal Runaway

The SEM micrographs and corresponding EDX elemental maps obtained from the top, penetration (middle), and bottom regions of the retained Cu current collector are presented in **Figure 44-46**. Clear differences in both residue morphology and elemental composition were observed between the three locations, indicating that the products formed during TR were not distributed uniformly throughout the cell.

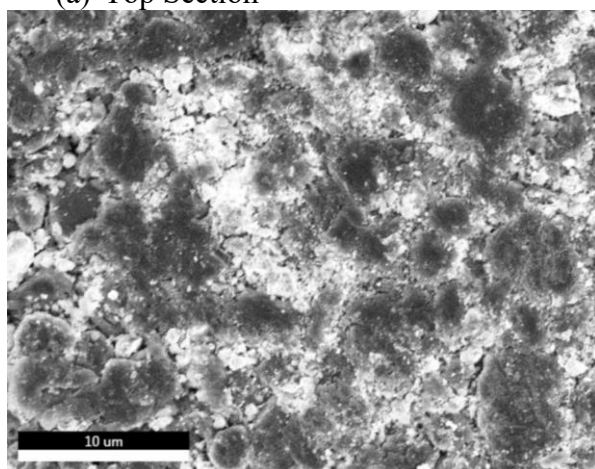
The top region of the current collector was a heterogeneous surface consisting of large, dark flake-like structures coated with finer, brighter particulate deposits. EDX analysis identified the flake-like structures as predominantly carbon-rich, while the brighter deposits were enriched in aluminum. Oxygen was distributed across much of the analyzed surface, whereas nickel and fluorine were detected within localized particles. Phosphorus was present only in trace amounts. The coexistence of carbonaceous flakes and Al-containing deposits suggests that this region consisted primarily of decomposed electrode material together with fragments originating from the Al current collector.

A very different morphology was observed at the penetration region. Unlike the top section, the residue consisted predominantly of fine, irregularly shaped particles with no distinct flake-like structures. EDX mapping revealed a comparatively lower carbon concentration but significantly greater oxygen, fluorine, and phosphorus concentrations. The enrichment of fluorine and phosphorus containing species is consistent with the presence of electrolyte decomposition products, suggesting that the region surrounding the NP site experienced more extensive electrolyte decomposition during TR. This observation is expected since the penetration region corresponds to the location of the internal short circuit, where the most intense thermal and electrochemical reactions occur.

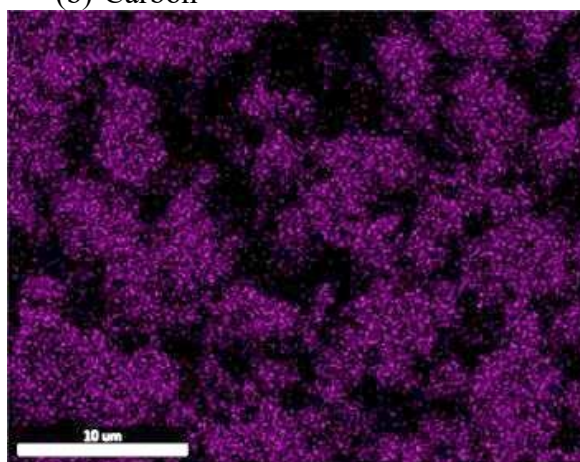
The bottom region had a morphology similar to that of the top section, consisting predominantly of large carbon-rich flakes. Carbon was the dominant element throughout the analysed area, while aluminum, nickel, oxygen, fluorine, and phosphorus were detected only in relatively low concentrations. Compared with the penetration region, the residue at the bottom of the cell appeared to be dominated by carbonaceous material, indicating fewer inorganic reaction products and less extensive electrolyte decomposition.

Overall, the SEM-EDX analysis demonstrates that the chemical composition of the post-TR residue varies considerably throughout the cell. Carbonaceous deposits were found to dominate the top and bottom regions, whereas the penetration region was enriched in oxygen, fluorine, and phosphorus containing species. These observations suggest that the thermal and chemical reactions occurring during NP-induced TR are highly localized, with the penetration region acting as the primary reaction zone while carbonaceous products are more prevalent in regions away from the point of mechanical abuse.

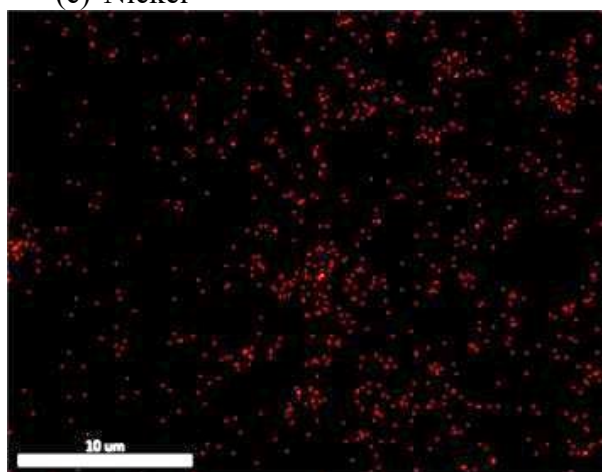
(a) Top Section



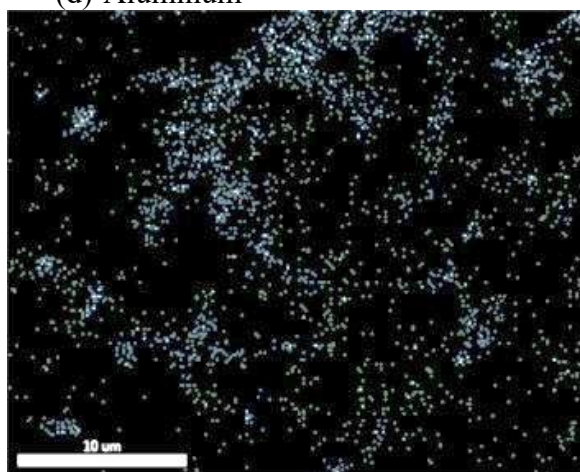
(b) Carbon



(c) Nickel

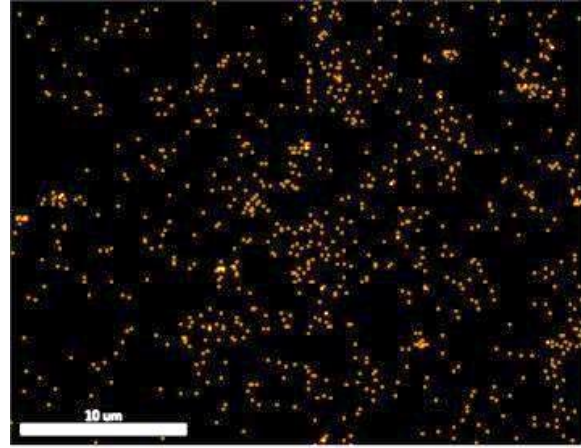
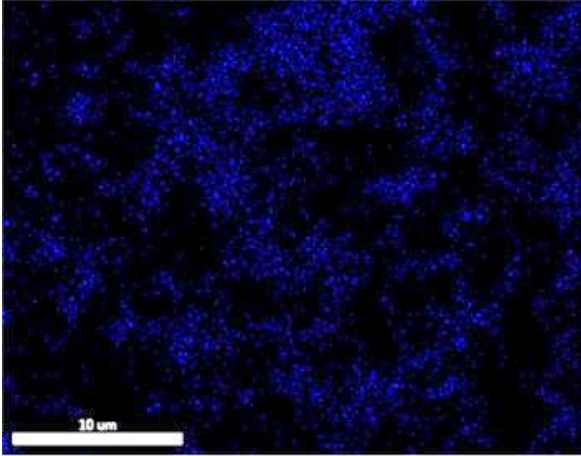


(d) Aluminum



(e) Oxygen

(f) Fluorine



(g) Phosphorous

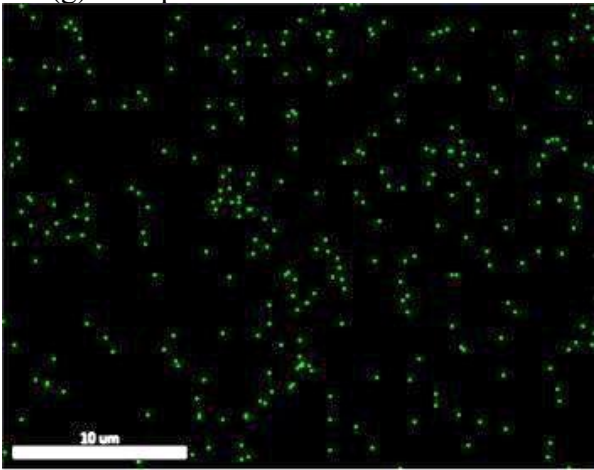
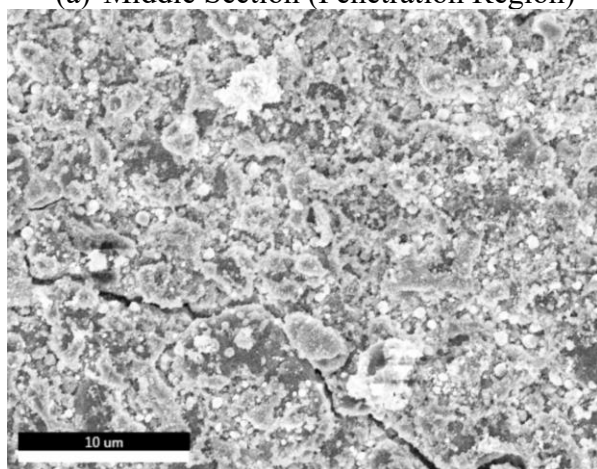
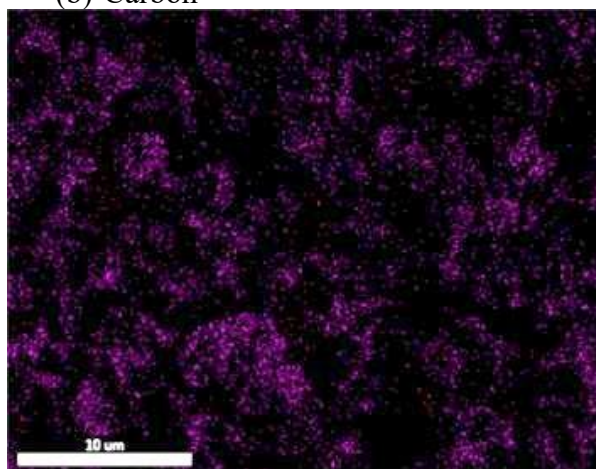


Figure 44: (a) SEM micrograph, and corresponding EDX elemental distribution maps of (b) carbon (C), (c) aluminum (Al), (d) oxygen (O), (e) nickel (Ni), (f) fluorine (F) and (g) phosphorus (P) for the top region of the retained Cu current collector following NP-induced TR

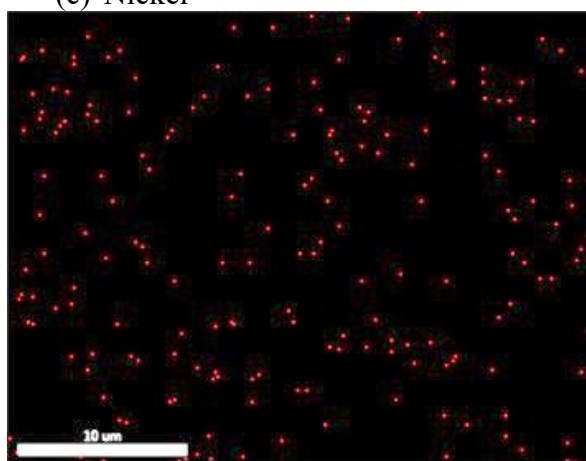
(a) Middle Section (Penetration Region)



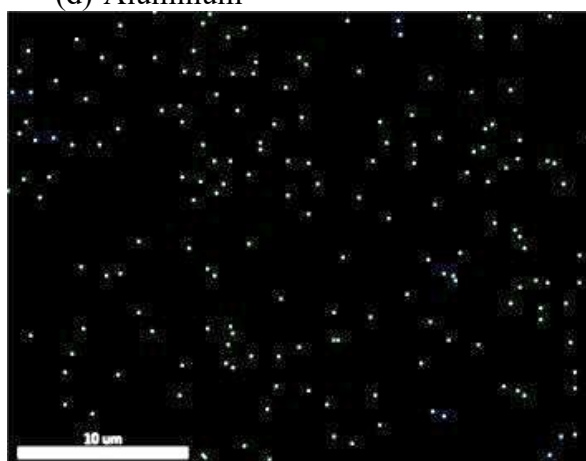
(b) Carbon



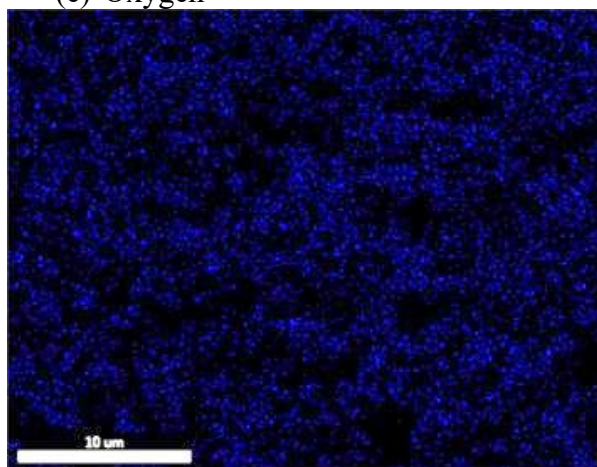
(c) Nickel



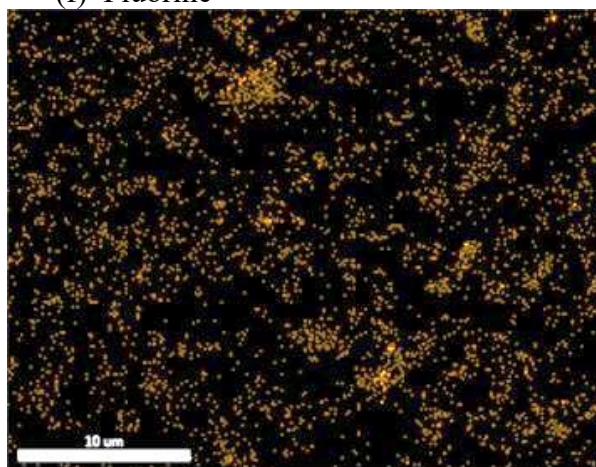
(d) Aluminum



(e) Oxygen



(f) Fluorine



(g) Phosphorous

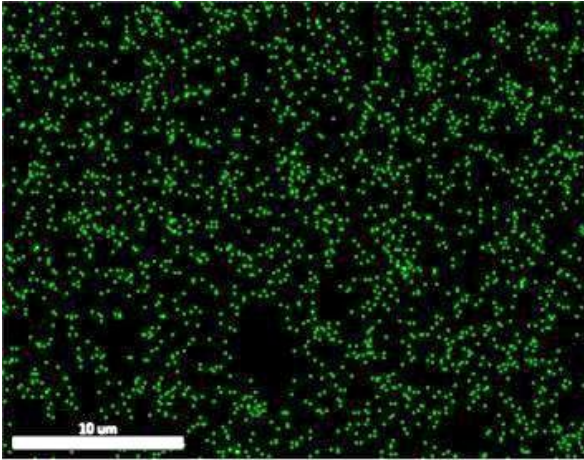
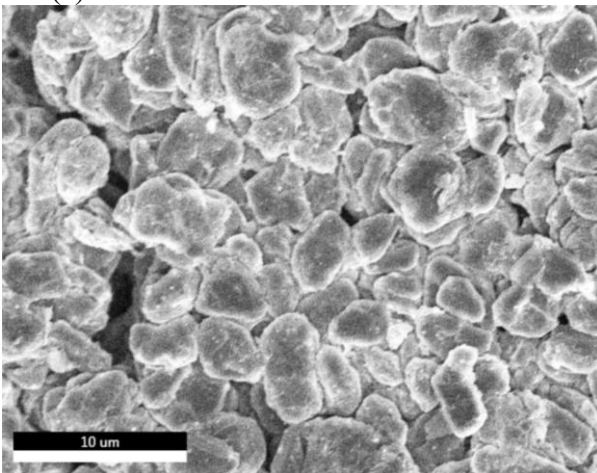
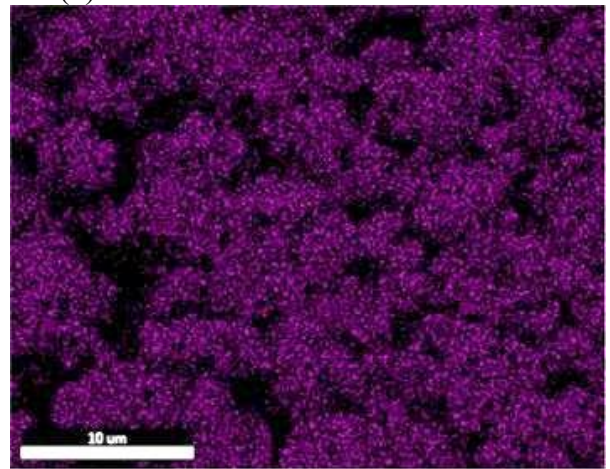


Figure 45: (a) SEM micrograph, and corresponding EDX elemental distribution maps of (b) carbon (C), (c) nickel (Ni), (d) aluminum (Al), (e) oxygen (O), (f) fluorine (F) and (g) phosphorus (P) for the penetration region of the retained Cu current collector following NP-induced TR

(a) Bottom Section

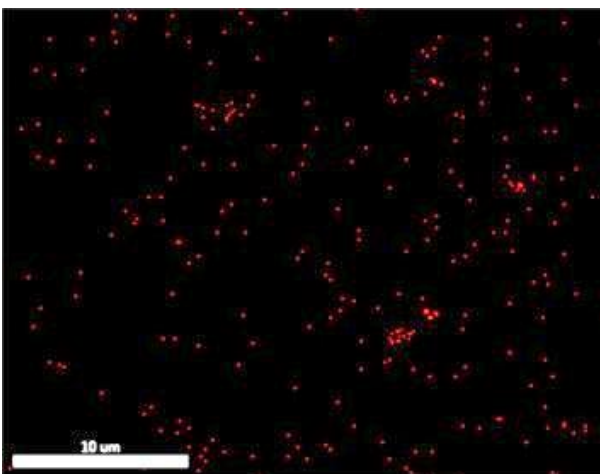


(b) Carbon

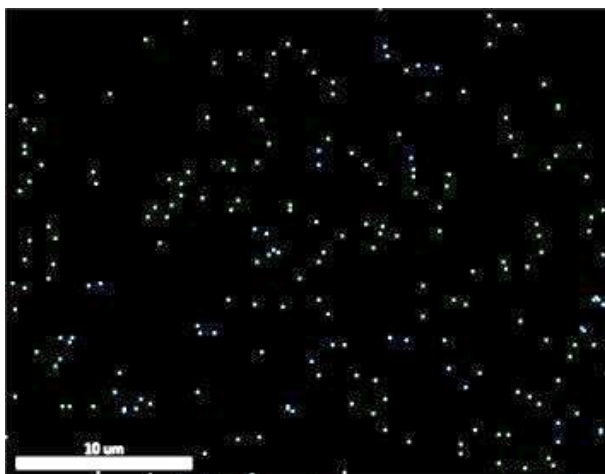


(c) Nickel

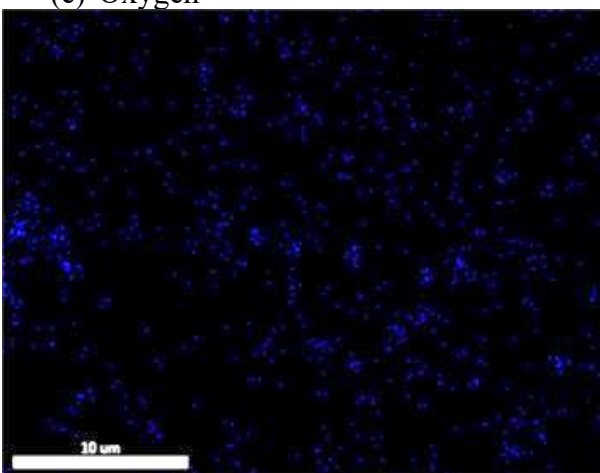
(d) Aluminum



(e) Oxygen



(f) Fluorine



(g) Phosphorous

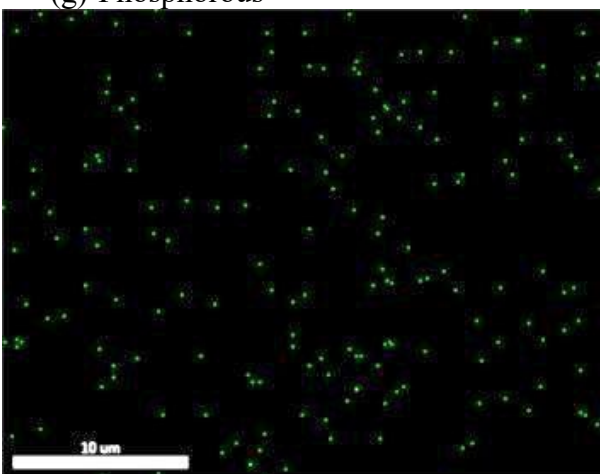
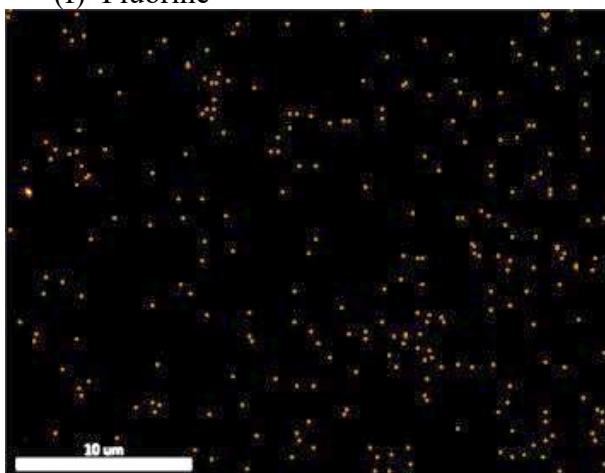


Figure 46: (a) SEM micrograph, and corresponding EDX elemental distribution maps of (b) carbon (C), (c) nickel (Ni), (d) aluminum (Al), (e) oxygen (O), (f) fluorine (F), (g) phosphorus (P), for the bottom region of the retained Cu current collector following NP-induced TR

6.2.4 XRD Results

The XRD pattern of the analyzed particles (**Figure 47**) revealed the presence of several crystalline phases associated with LIB materials and TR reaction products. Nickel- and cobalt-containing phases were identified, consistent with cathode-derived materials originating from fragmentation and ejection of electrode components during TR. In addition, lithium cobalt oxide (LCOx) and cobalt sulfate (CoSO_4) phases were detected, suggesting the formation and persistence of metal oxide and sulfate species under the high-temperature and chemically reactive conditions characteristic of TR.

Silicon- and silica-based crystalline phases (Si and SiO_2) were also identified in the XRD spectra. SEM-EDX analysis revealed the presence of a localized Si-rich particle within one analysed region; however, silicon was not consistently detected across the remaining samples and mapped regions. This suggests that silicon-containing species were present within the emitted PM but were distributed heterogeneously throughout the collected particles. Potential sources include silicon-containing anode additives, separator coatings, or other cell components, although the limited spatial occurrence of Si prevents definitive attribution to a specific origin.

Sulfur-containing phases (CSO_3) might originate from sulfur-based additives that are typically used to improve anode performance [99], or from secondary reaction products generated during TR. The elevated temperatures and chemically reactive environment associated with TR can promote reactions involving electrolyte decomposition products and metallic species, leading to the formation of sulfate-containing compounds such as CoSO_4 .

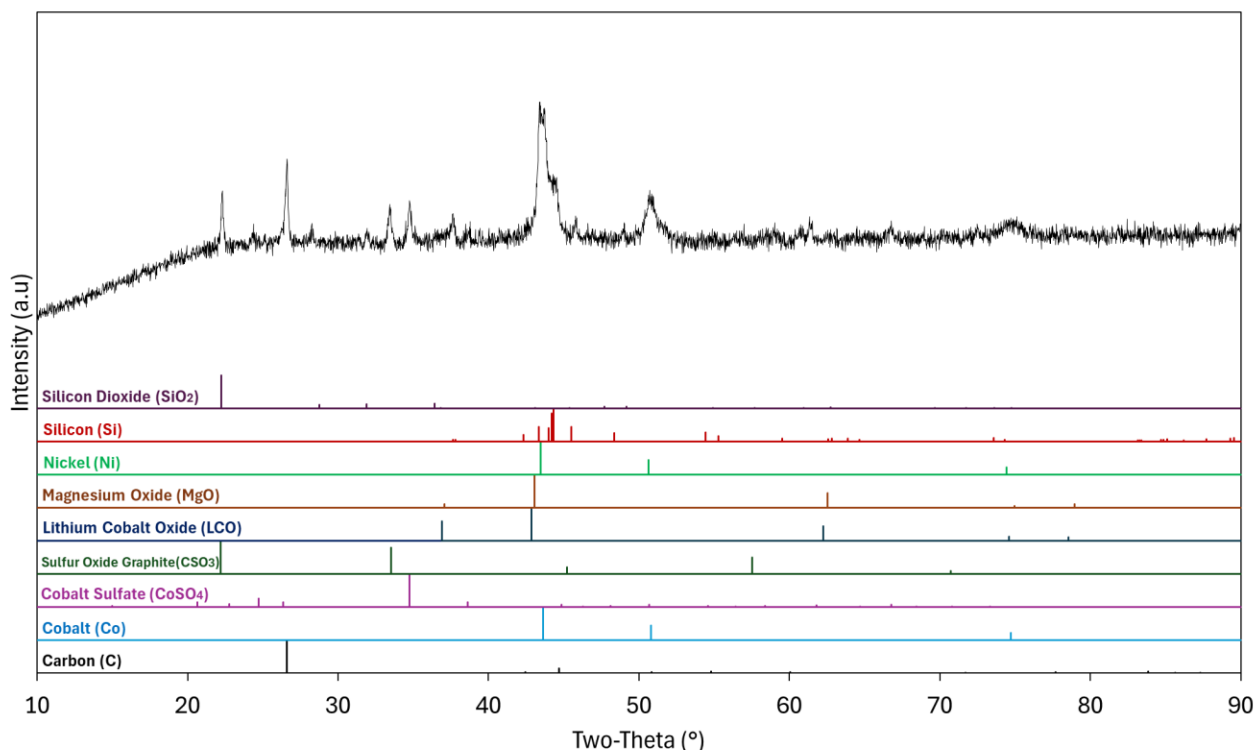


Figure 47: XRD pattern of mechanically ground TR particles collected from an LG-HG2 cell following NP-induced TR. Reference patterns corresponding to the identified crystalline phases are shown beneath the experimental diffractogram

6.2.5 Summary

Overall, the particle characterization results demonstrate that the TR ejecta generated during NP of NMC 18650 cells consists of a heterogeneous mixture of carbonaceous residues, metallic particles, and fragmented electrode materials. PSD analysis revealed that the emitted PM was predominantly composed of submicron particles, while SEM observations identified spherical, irregular, agglomerated, and flake-like morphologies. EDX and XRD analyses confirmed the presence of battery-derived metallic species and crystalline phases associated with internal cell components.

Post-TR examination of the disassembled cell further showed that substantial portions of the Cu current collector remained intact, whereas the separator, electrode coatings, and Al current collector underwent extensive degradation. SEM-EDX analysis of residues deposited on the retained Cu current collector revealed clear spatial variations in composition of species. These observations suggest that NP-induced TR is governed by localized reactions, causing non-uniform formation and deposition of decomposition products throughout the cell.

Collectively, these findings suggest that TR particulate emissions are produced through a combination of fragmentation, melting, condensation, and combustion-driven processes, resulting in a complex particulate mixture with implications for environmental contamination and post-fire exposure.

6.2.6 Experimental Limitations and Qualitative Uncertainty

The findings of this study should be interpreted in consideration of several experimental limitations and sources of qualitative uncertainty. A relatively small number of repeated experiments was conducted under each test condition, particularly for the low-temperature tests, and some temperature records were excluded because of thermocouple displacement. The limited sample size restricts statistical quantification of variability and prevents precise determination of an SOC or temperature threshold for thermal runaway (TR). Furthermore, the comparison of commercial cells was qualitative because chemistry, capacity, form factor, internal construction, and SOC were not independently controlled.

The assigned SOC values were estimated from an experimentally determined voltage–capacity relationship. Cell-to-cell differences in capacity, aging, and relaxation behaviour may therefore have caused the actual SOC to differ slightly from the reported values. For the low-temperature experiments, the cells warmed during transfer and installation, and their internal temperatures at the time of penetration were not directly measured. The surface thermocouple readings of approximately 7 °C and 1.3 °C also differed from the –30 °C and –40 °C chamber setpoints. In addition, nail temperature was not controlled, and residual heating of the nail may have influenced ignition behaviour in successive tests.

The measured temperatures were sensitive to the mechanical configuration. Small variations in cell alignment, displacement during penetration, venting direction, and flame trajectory influenced thermocouple exposure. Because each thermocouple provided a localized measurement, flame

impingement, probe contact, and ejecta direction could affect the measured peak temperatures and heating rates. The emission temperature was measured after gases travelled through the sampling line and therefore does not represent their temperature at the cell outlet. Visual determinations of ignition and flame extinction were also subject to camera resolution and obstruction by smoke.

The particulate characterization represents material collected from LG-HG2 cell tests from the test bed. This method captured only the fraction of particles deposited and not the complete airborne aerosol. Consequently, the SEM-derived particle size distribution (PSD) should not be interpreted as the size distribution, mass concentration, or emission rate of the entire airborne particulate population.

Physical and chemical transformations may also have occurred after particle emission. Hot particles were exposed to oxygen, atmospheric moisture, and combustion gases during transport, deposition, and storage. Oxidation, hydrolysis, surface reactions, volatilization or condensation of semi-volatile species, and particle agglomeration could therefore have altered the measured composition and size. Fluorine- and phosphorus-containing electrolyte residues may be particularly susceptible to reactions with atmospheric moisture. The SEM-EDX and XRD results consequently describe the collected post-emission residue and may not fully represent particles at the instant of formation.

Additional analytical uncertainty resulted from the carbon tape contribution to the EDX carbon signal, the use of aluminum stubs, the analysis of selected SEM regions, and the qualitative classification of particle morphologies. The two-dimensional equivalent circular diameter does not represent the real size of the particle, while segmentation thresholds, overlapping particles, agglomerates, and particles below the imaging resolution may affect the calculated distribution. XRD primarily identifies crystalline phases and may not detect amorphous or poorly crystalline products. Therefore, the results provide strong qualitative evidence of the observed trends and particulate formation pathways, but absolute values, inter-cell comparisons, and exposure-related interpretations should be generalized with caution.

Chapter 7 Conclusions and Recommendations

Nail penetration (NP) experiments conducted on LG-HG2 18650 cells revealed that state-of-charge (SOC) has a significant influence on thermal runaway (TR) initiation and severity. Cells tested at 100%, 95%, and 77% SOC all underwent immediate TR following NP, whereas the 68% SOC cells did not ignite and instead produced a sustained smoke plume from the penetration site. In general, higher SOC conditions resulted in more severe TR events characterized by higher temperatures, rapid ignition, and increased combustion intensity. However, variability between repeated tests was observed, particularly at 77% and 68% SOC, indicating that TR behaviour is influenced by both the stored energy content of the cell and the stochastic nature of failure initiation during NP. These findings confirm that increasing SOC increases both the likelihood and severity of TR during mechanical abuse and highlight the importance of SOC management as a battery safety mitigation strategy.

NP experiments conducted on cells preconditioned to -30 °C and -40 °C demonstrated that initial cell temperature significantly influences TR behaviour. Although TR was observed under all low-temperature conditions investigated, distinct differences in ignition behaviour were observed. Cells preconditioned to -30 °C underwent immediate TR upon penetration, whereas cells preconditioned to -40 °C exhibited delayed ignition in two of the three test runs. In these cases, ignition occurred several seconds after NP and was associated with nail retraction and the release of flammable electrolyte and gases from the cell. The delayed response suggests that reduced ionic conductivity at subzero temperatures limits the heat generation required for immediate TR initiation. In addition, low-temperature preconditioning reduced TR severity, resulting in lower surface and ejecta temperatures compared to ambient-temperature tests. Nevertheless, the results indicate that low temperature alone does not eliminate the risk of TR following severe mechanical abuse.

SEM characterization of particulate matter (PM) generated during TR revealed that the emitted particles consisted of a heterogeneous mixture of particles with varying sizes, morphologies, and elemental compositions. Particle size distribution (PSD) analysis showed that the emitted particles were predominantly within the submicron size range, with a median particle diameter (D50) of approximately 0.1 μm . Several distinct particle morphologies were identified, including spherical, flake-like, irregular, and agglomerated structures. EDX analysis confirmed the presence of carbon-

rich particles together with metallic elements associated with battery components, while XRD analysis further verified the presence of crystalline degradation products generated during TR. The characterization approach employed in this work enabled the correlation of particle size, morphology, and composition while preserving the native structure of the collected particles.

Post-TR examination of the disassembled cells showed that substantial portions of the Cu current collector remained intact, while SEM-EDX analysis revealed clear spatial variations in residue composition throughout the cell. Carbon-rich residues were predominantly observed in the upper and lower regions of the cell, whereas oxygen, fluorine, and phosphorus-rich species were concentrated near the penetration region, suggesting localized electrolyte decomposition following NP. Collectively, these findings provide new insight into both the composition of emitted PM and the distribution of decomposition products remaining within the failed cell following TR.

The experimental methodology developed in this work demonstrates that combining thermal measurements with detailed post-TR material characterization provides valuable insight into the mechanisms governing NP-induced TR. The findings contribute to the understanding of both the thermal behaviour and particulate products generated during mechanical abuse of LIBs and may support the development of improved battery safety assessment and mitigation strategies.

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