MULTIPHYSICS MODELING FOR SAFE BATTERIES USING LS-DYNA

G. Di Mauro[1], M. Guida[1], G. Olivares[2], L. M. Gomez[2]

[1]Department of Industrial Engineering, University of Naples Federico II, Naples, IT
[2]Jerry Moran Center for Advanced Virtual Engineering & Testing (AVET), National Institute for Aviation Research (NIAR), Wichita State University (WSU), Kansas, US

Abstract

Within the global push towards environmental sustainability, lithium-ion batteries are the dominant power source for various applications due to their high energy density. Therefore, aviation industry is increasingly investigating electrification as a potential solution to reduce emissions and combat climate change. However, widespread adoption is hindered by safety concerns arising from potential failure scenarios. A comprehensive understanding of these failure mechanisms is paramount for advancing lithium-ion battery safety and paving the way for a more sustainable aviation future.

This paper presents a critical review of the current state of the art on lithium-ion battery failure mechanisms under diverse abuse conditions, encompassing thermal, electrical, and mechanical responses. It underscores the significance of multiphysics simulations, integrating structural, electrical, and thermal responses, in the design of inherently safer lithium-ion batteries.

Furthermore, the paper focuses on Structural Batteries, a novel technology with the potential to revolutionize electric air transport. Structural Batteries offer a compelling solution by seamlessly integrating energy storage and load-bearing capabilities. This integration has the potential to alleviate the weight penalty associated with conventional battery packs in electric aircraft, thereby extending range and payload capacity.

The paper analyzes the challenges and future directions for structural battery research. It emphasizes the pivotal role of advanced Finite Element Analysis simulations in modeling the behavior of structural batteries under abuse conditions. These simulations can be instrumental in predicting internal short circuit occurrence, a critical safety concern. By leveraging such predictive capabilities, the development of safer and more efficient structural batteries can be expedited, paving the way for a more sustainable future for electric aviation.

Keywords: batteries, airworthiness requirements, certification by analysis, internal short circuit, thermal runaway

1. Introduction

The modern society is facing the critical challenges of the environmental pollution and the need to reduce the reliance on traditional combustion energy sources. Recent technological breakthroughs have enabled the conversion of nuclear, wind, and solar energy into electrical power efficiently and with reduced environmental impact [1]. The coming era of electric energy is changing the energy source of vehicle from fossil fuels to electrochemical energy storage systems [2], thereby changing the propulsion system from engine to motor. Electric vehicle (EV), including hybrid electric vehicle (HEV) and pure battery electric vehicle (BEV), is the actual demonstration of this transformative process.

Lithium-ion batteries (LIBs) have emerged as the dominant rechargeable power source due to their exceptional energy density, high voltage output, and minimal self-discharge. This versatility positions them favourably across diverse applications, from portable consumer electronics to large-scale electric vehicles (EVs) and even airplanes.

However, LIBs possess inherent limitations that impede their optimal utilization. Their operational temperature range and charge/discharge rates are comparatively narrow, as documented in various studies [3-7]. Elevated temperatures exacerbate battery degradation, leading to diminished lifespan. Furthermore, exceeding these design parameters can trigger uncontrolled self-heating, a phenomenon known as thermal runaway. Thermal runaway carries the significant risk of igniting surrounding materials, potentially escalating into catastrophic events.

While the failure rate of LIBs is considered exceptionally low under recommended operating and storage conditions, unforeseen circumstances can drastically elevate this risk. Factors such as overcharging, exposure to extreme temperatures, and mechanical damage can significantly increase the probability of failure. Despite the integration of safety features in commercially available LIBs, several high-profile incidents involving battery failure have been documented [8]. These accidents have resulted in severe consequences for both cell manufacturers and companies that incorporate LIB technology into their products.

The concerning frequency of catastrophic accidents involving LIBs has spurred regulatory bodies to implement stricter controls governing their transportation and storage. As a prominent example, the International Civil Aviation Organization (ICAO) has enacted a ban on the transport of LIBs as cargo on passenger airplanes. Even for cargo-only aircrafts, stringent regulations mandate a state of charge (SOC) below 30% for transported LIBs [9].

While the demand for ever-smaller and lighter electronic devices continues unabated, it concurrently drives the relentless pursuit of higher energy density in LIBs. This trend, however, hinders the potential to exacerbate the severity of battery failures. A comprehensive understanding of the various LIB failure mechanisms is crucial for the development of safer and higher-energy density battery technology.

LIB abuse can be broadly classified into three primary categories: thermal, electrical, and mechanical. Thermal abuse encompasses situations like overheating [10] and direct fire exposure. Electrical abuse includes overcharging [11-17], over-discharging [18], and internal/external short circuits [19]. Mechanical abuse scenarios can occur during crash, penetration, or bending load conditions [20-22].

Physical abuse, which can manifest as penetration, pinching, or bending, can lead to a potentially catastrophic situation called Internal Short Circuit (ISC). This occurs when the separator, a critical component that physically separates the anode and cathode, becomes compromised. Penetration by a sharp object, separator fracture, or even significant electrode deformation can all lead to direct contact between the anode and cathode. Electrical abuse, particularly overcharging, can induce the formation of lithium dendrites within the battery. These needle-like structures can grow and eventually pierce the separator, again causing an ISC. Even thermal abuse, independent of physical damage to the separator, can trigger ISC. The intense heat can lead to exothermic reactions within the anode and/or cathode materials, generating further heat and potentially causing a thermal runaway event. A schematic representation of these LIB abuse conditions is provided in Figure 1.

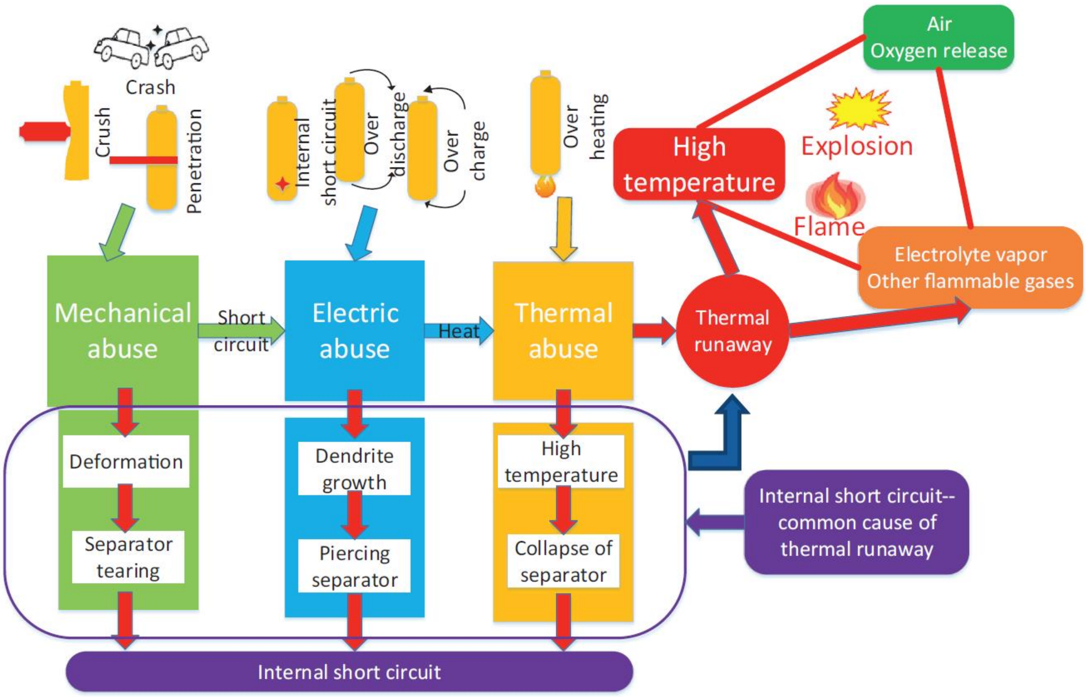


Figure 1 - Schematic of LIB abuse conditions [8].

Therefore, it is well-established that internal short circuit is the most prevalent and fundamental trigger for catastrophic thermal runaway events in LIBs, regardless of the initial abuse type.

Understanding the complex interplay of physical phenomena within LIBs is fundamental for safety purposes. These phenomena occur across different time and length scales, ranging from individual particles to entire electrode structures, cells, and even battery packs.

The intricate interplay encompasses:

- Electrochemical reactions occurring within the active materials of the anode and cathode.
- Electron transport through the current collectors within the cell.
- Heat generation, resulting from charge and discharge cycles.
- Chemical interactions on the electrolyte and electrode surfaces.
- Mechanical deformations, eventually due to applied external forces.
- Coupling effects due to the interplay of these various multiphysics responses.

Therefore, investigation of these phenomena has become fundamental in the research field. Computational models have emerged as a powerful tool for studying multiphysics algorithms, offering valuable insights for the design of inherently safer LIBs. Furthermore, ongoing research advancements, encompassing both experimental and numerical approaches, are fundamental to achieving a comprehensive understanding of the multiphysics nature governing these critical phenomena within LIBs [23]. To clarify the underlying mechanisms of LIB failure under crushing or impact loading, and to improve the accuracy of numerical predictions, researchers have focused on various structural levels within the battery.

Pioneering work by Wierzbicki et al. [24, 25] and Greve and Fehrenbach [26] involved conducting quasi-static tests on both cylindrical and pouch cells under varying loading and boundary conditions. These studies revealed the crucial relationship between the ISC onset and the characteristics of the mechanical response. Based on these findings, Wierzbicki et al. [27-29] developed homogenized finite element (FE) models that demonstrated good agreement with experimental observations.

Internal Short Circuit occurrence is striclty linked to the integrity of the separator layer within batteries, which has the crucial function of avoiding direct contact between the electrode layers. Sheidaei et al. [30] investigated the tensile behaviour of single-layer polypropylene separators, in both dry and electrolyte-saturated conditions. Their work highlighted the significant reduction in the separator mechanical properties when exposed to electrolyte solutions. Cannarella et al. [31] furthered this research by presenting a straightforward method for measuring the compressive and tensile mechanical properties of LIB separators. Leveraging these results, Gor et al. [32] established a material model capable of predicting the elastic response of separators while incorporating the strain-rate effect.

Lai et al. [33,34] and Ali et al. [35] undertook a series of combined experimental and computational investigations on representative volume element (RVE) specimens extracted from prismatic graphite/LiFePO4 pouch cells. This approach enabled them to analyse the development of localized deformation patterns within the battery under in-plane compression loading conditions. Their findings suggested that the LIB anode and cathode active material coatings exhibit minimal load-carrying capacity, prompting their modeling as foam materials. Similarly, Avdeev and Mehdi [36] employed high-speed cameras to experimentally characterize the non-linear mechanical deformation of cylindrical LIBs under lateral impact. They subsequently developed a homogenized finite element model to estimate the impact time during drop tests.

Wang et al. [37] proposed a simplified analytical model, employing a clay-like analogy, to characterize the radial compression response of cylindrical battery cells. In contrast, Xu et al. [38-41] focused on investigating the mechanical integrity of cylindrical battery cells under various loading scenarios (e.g., nail penetration, compression, and bending). Their work culminated in the establishment of a rate-dependent and SOC-dependent homogenized model for cylindrical cells.

Researchers such as Maleki et al. [42,43] conducted mechanical abuse tests on battery cells under specific loading conditions, including pinch, penetration, and bending. These studies aimed to acquire mechanical response data and analyse the influence of various factors on the development of ISC. Doughty and Pesaran [44] further compiled a comprehensive review of mechanical abuse tests conducted on battery cells, modules, and packs. Hatchard et al. [45] introduced a novel "smart nail" penetration test method for LIBs. This method incorporates thermocouples embedded within the nail tip to collect real-time temperature data at the point of penetration. Lamb and Orendorff [46] highlighted the significant variability observed in test results obtained from mechanical abuse testing, emphasizing the sensitivity to specific test conditions.

While significant research has focused on the mechanical response of individual battery cells under abuse conditions, investigations at the battery module level and above have primarily focused on thermal behaviour and electrical management.

Lamb et al. [47] investigated the propagation of thermal runaway within small battery modules containing different cell types and electrical configurations. Their study employed a "hard" internal short circuit induced by mechanical nail penetration in a single cell. Similar work by Feng et al. [48] utilized nail penetration to trigger a short circuit and subsequently analyse thermal runaway in a large-format lithium-ion battery module comprised of six prismatic cells. Their findings highlighted the dominant role of heat transfer through the battery shell in governing thermal runaway propagation. Based on these results, Zhao et al. [49] proposed an electrochemical-thermal model informed by nail penetration tests. Their study demonstrated the effectiveness of a hydrogel cooling system in mitigating battery thermal runaway.

Shifting focus to electric vehicles (EVs), Xia et al. [50] conducted a pilot study on the safety and protection of battery packs against ground debris impact. This study employed simulations to assess localized indentation within the battery pack, consisting of cylindrical cells. The research analysed the deformation and damage progression of individual battery cells within the pack, alongside the influence of fractures in shield plates constructed from various metal materials.

As evidenced by the previous references, the ever-expanding utilization of lithium-ion batteries across diverse applications underscores the critical need for advanced simulation tools. These tools should possess the capability to predict the combined structural, electrical, electrochemical, and thermal response of batteries subjected to abuse conditions. Therefore, the integration of such simulation tools within the product development process becomes crucial. The resultant data holds immense potential for creating highly optimized battery designs and achieving virtual verification of these designs before physical prototyping is undertaken.

These considerations become even more important when dealing with Structural Batteries (SBs), novel technologies deeply investigated in the research scenario. They hold the immense potential of electrifying the air transport sector, since they combine electrical-energy-storage and load-bearing capabilities.

It is evident that aircraft relying exclusively on conventional battery packs are subjected to design limitations. The weight penalty associated with storing the required electrical power triggers a detrimental effect on the overall aircraft weight, due to the limited energy-to-mass and energy-to-volume ratios of conventional batteries, thus hindering flight range and payload capacity [51].

This justifies the ongoing research efforts aimed at improving these performance metrics for electric aircraft, both prototypes and production models, belonging to very-light and ultralight aviation categories [52], in which the contribution of battery packs on the aircraft overall weight is reduced. For instance, Pipistrel Velis Electro is the only commercially certified full-electric aircraft [53] and it belongs to the very-light-aircraft category, whereas in General Aviation no full-electric aircraft is commercially available to date.

Structural Batteries enable the possibility to mitigate the weight penalty associated with traditional battery packs by combining energy-storage and load-bearing capabilities. Therefore, research activity on SBs is rapidly expanding. Studies by Adam et al. [54] suggest that SB integration as energy storage devices within aircraft structures could achieve a range extension of 11-66% under ideal conditions. Recent research focuses on balancing mechanical and energy storage performance. For instance, Schutzeichel et al. [55] investigated carbon fibers as structural anodes, while Leijonmarck et al. [56] explored their use as negative electrodes, and Shirshova et al. [57] analyzed bi-continuous liquid-epoxy systems for stiff structural solid electrolytes. These advancements pave the way for optimizing SBs' multifunctional capabilities. Scholz et al. [58] demonstrated that SBs with a minimum energy density (one-third to one-half of conventional batteries) could replace entire propulsion batteries in small electric aircraft. Additionally, Karadotcheva et al. [59] investigated SBs' potential to improve fuel efficiency and reduce greenhouse gas (GHG) emissions in A320-like aircraft configurations. Nguyen et al. [60] explored the feasibility of embedding SBs in the cabin floor panel of an A220-like aircraft, demonstrating their potential to power in-flight entertainment systems. Riboldi et al. proposed a detailed preliminary design for a CS-23-compliant hybrid electric general aviation aircraft incorporating SBs [61].

Despite promising forecasts, several challenges remain. These include material configuration and functionalization [62], optimization strategies for balancing structural and electrochemical properties [63, 64], environmentally friendly manufacturing processes, large-scale production methods, and life cycle analysis [65]. Safety, in particular, is a critical concern. Since SBs are likely lithium-based, they share the inherent safety risks of conventional batteries. Moreover, their structural load-bearing role makes addressing potential failure conditions even more sensitive.

The aim of this article is to support the use of advanced Finite Element Analysis (FEA) to model the mechanical, thermal and electrochemical behaviour of Structural Battery composites when subjected to abuse load for ISC occurrence predictions. Firstly, taking as a reference the experimental activities performed in [66], a numerical model validation (from a structural point of view) is performed on a SB coupon subjected to tensile test. The same stands for a carbon fiber (CF) laminate coupon, with and without embedded Structural Batteries, to evaluate the expected decrease in structural performance. Following the validation process and a comprehensive review of the strategies available in LS-Dyna software for modeling the multiphysics (structural, thermal and electrochemical) response of batteries under abuse load conditions, a case study is presented. This case study involves the application of an mechanical abuse loading on a SB, highlighting the difference in its response when integrated in a CF laminate.

2. Tensile Test Model Validation

Structural batteries represent a promising solution for enhancing the electrical energy storage capabilities of aircraft. These multifunctional components, fabricated similarly to composite materials already employed in many aircraft, hold the potential to replace stress-bearing parts typically made from metal alloys or carbon fibers [67-71].

Meaningful is the study performed by F. Laurin et al. [66] within the CleanSky2 THT project SOLIFLY. In particular, the envisaged SB concept is the Reinforced Multilayer Stack (RMS), which configuration is extensively explained in [72]. Figure 3 illustrates the conceptual cell geometry for the investigated RMS approach. Each cell is designed with a total thickness of approximately 210 μm, aligning with the typical ply thickness used in composite laminates. To mitigate the risk of electrical shorting at the electrode corners, the electrolyte layer has been designed to be slightly larger than the electrodes themselves. RMS battery cell specimens with an in-plane size of 150 mm x 20 mm were subjected to tensile tests. The experimental test set-up, along with the adopted output measurement instrumentation, is showed for clarity in Figure 4. The tensile tests were performed at a constant displacement rate of 0.5 mm/min until failure, reached at a failure stress of 36.5 MPa.

Concerning the laminate in which the Structural Batteries have been integrated, it was decided to consider AS4/8552 unidirectional plies, widely used in the aeronautical industry. The mechanical properties of the material, taken from the literature [66, 73-75], are schematically reported in Table 1.

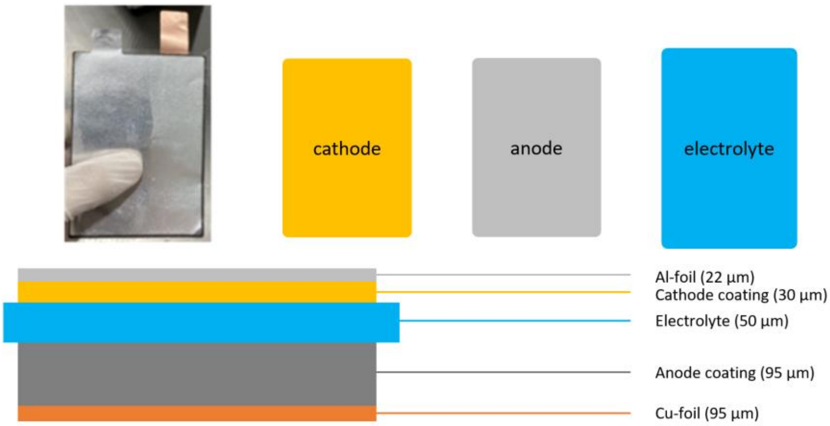


Figure 2 - RMS battery cell with the detail of its through-the-thickness configuration [65].

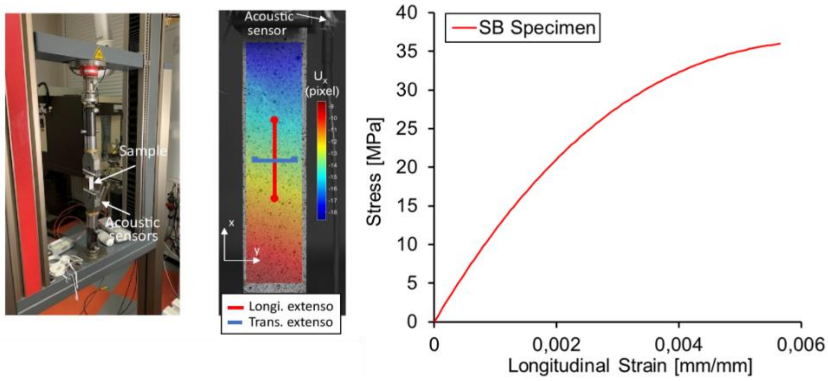


Figure 3 - Electromechanical testing machine, measured displacement field and associated virtual extensometers (left), stress/strain curves for the tested RMS cell specimens (right) [65].

Table 1 - Mechanical properties of AS4/8552 unidirectional ply [65, 72-74].

Properties	AS4/8552	Properties	AS4/8552
E_{11}	134.0 GPa	X_t	1950 MPa
E_{22}	10.0 GPa	Y_t	88 MPa
G_{12}	4.9 GPa	Y_c	-250 MPa
v_{12}	0.3	S_c	110 MPa

In order to check the relevance of these material data, a quasi-isotropic $[(45/90/-45/0)_2]_s$ laminate has been manufactured, from which specimens measuring 200mm x 25mm x 2.92mm have been obtained. Then, it was decided to consider a laminate with the same stacking sequence, in which six RMS battery cells have been integrated only in the central 90 plies and ±45 plies, thus resulting in two modules (each one containing three cells), as schematically reported in Figure 5. Finally, a tensile test campaign has been performed on the mentioned specimens to evaluate the decrease in the mechanical performances when SBs are embedded into the laminate structure. The results, along with the test set-up are shown in Figure 6.

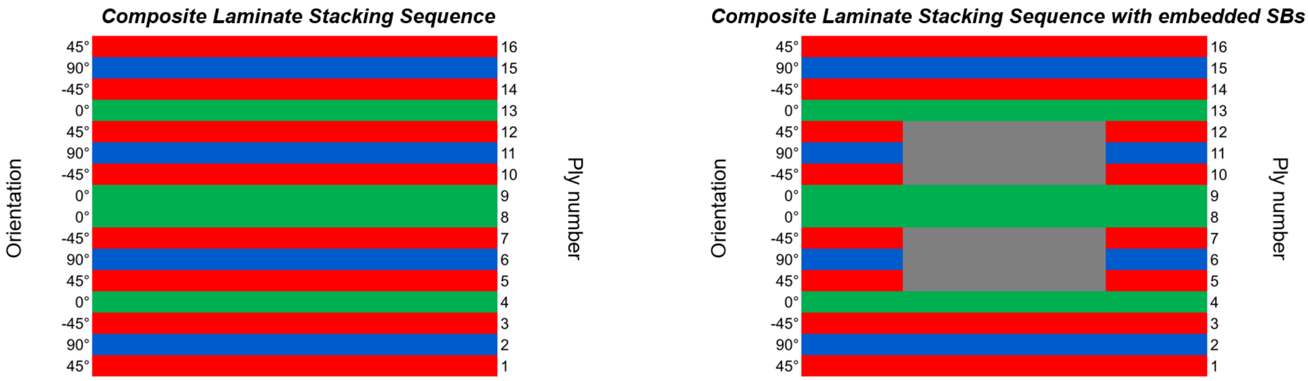


Figure 4 – Stacking sequence for reference laminate (left) and laminate with embedded SBs [65].

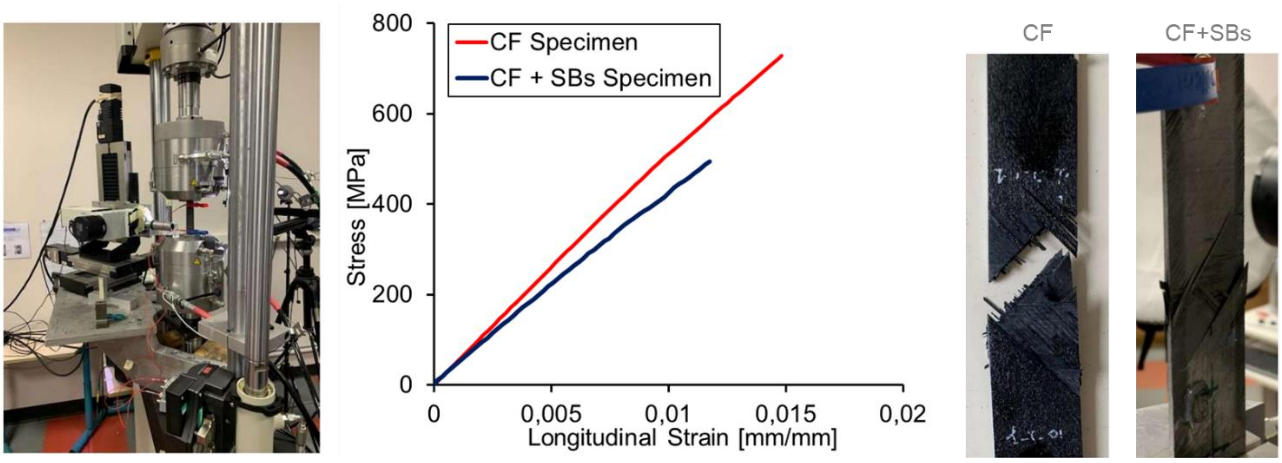


Figure 5 - Hydraulic testing machine adopted for testing (left), comparison on the CF laminates of experimental stress/strain curves (center) and failure patterns [65].

Based on those experimental results, a numerical simulation campaign was undertaken utilizing the commercial solver LS-Dyna. Such numerical campaign aimed to well establish the material model for both the RMS battery cell and the composite laminate. Initial focus was dedicated on replicating the tensile test conducted on a single RMS cell. Two distinct discretization strategies were employed, the first one adopting two-dimensional (2D) elements on the specimen's midplane, while the second strategy employing three-dimensional (3D) elements covering all the specimen thickness. Both

approaches maintained a consistent mesh size of 1mm. Notably, the simulations solely considered the free gauge length of the specimen, excluding the gripping regions. Consequently, the nodes on the top edge were clamped, whereas the nodes on the bottom edge were subjected to a prescribed displacement along the longitudinal axis. A schematic representation of the implemented boundary conditions is presented in Figure 7, along with a focus on the two adopted discretization strategies.
The same assumptions have been considered both for the reference CF laminate specimen and the one with embedded SBs, as shown in Figure 8. Significantly, both for the CF laminate and the one with integrated SBs, the component pertaining to the laminate itself was switched to part composite. This was done to eventually accommodate the inclusion of a distinct material model within the stacking sequence of the laminate.

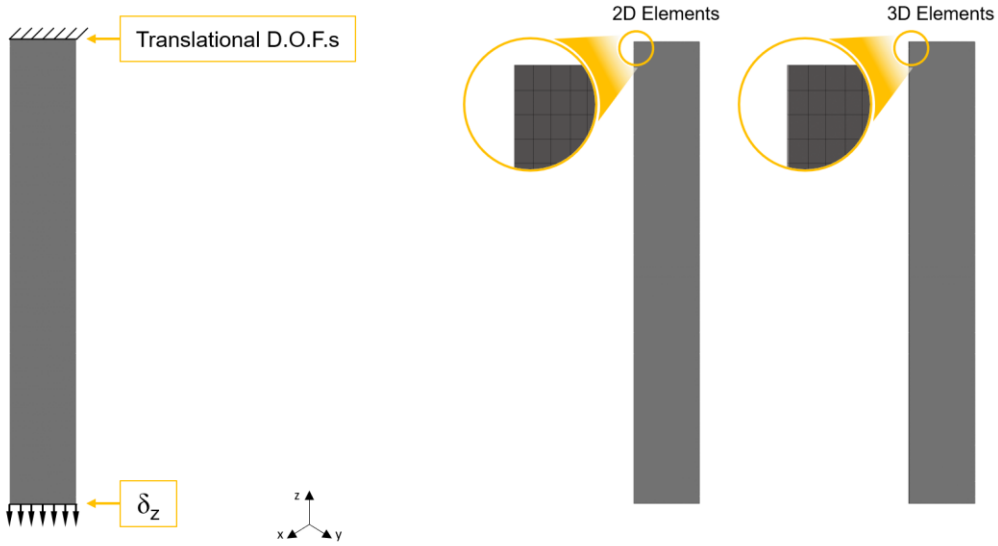


Figure 6- Adopted boundary conditions for tensile test simulations (left) with a focus on the discretization strategies for the RMS cell (right).

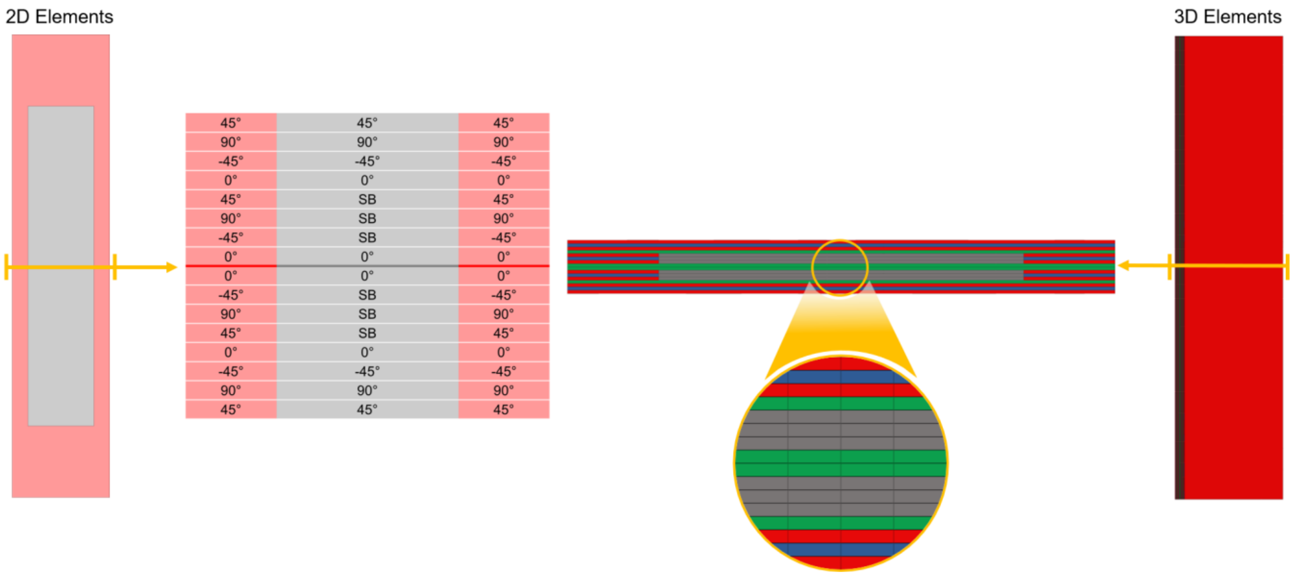


Figure 7 – Adopted discretization strategies for the CF laminate with embedded SBs.

The numerical models have been compared with experimental results in terms of stress-strain curves, which is the most relevant information gathered from reference [66]. As shown in Figure 9 a good agreement has been reached for the adopted material models to be validated, especially when dealing with the model including 3D elements, which is the one adopted in the following application.

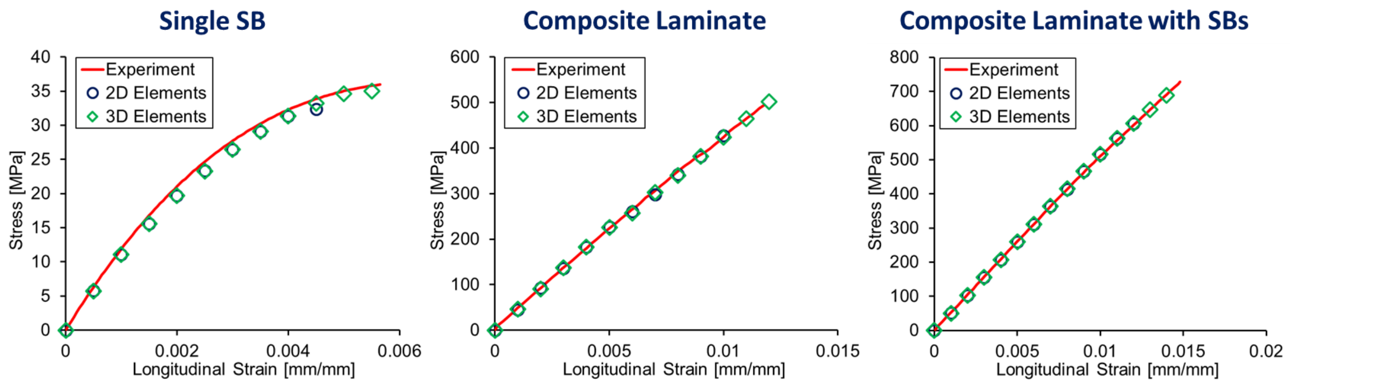


Figure 8 - Experimental-numerical comparison of stress-strain curves: Single Structural Battery (left), Composite laminate (center), Composite laminate with embedded SBs (right) specimens.

3. ISC Simulations on Structural Batteries

Upon confirming the mechanical properties of both the structural battery and the CF laminate material models, the numerical model was deemed fit for application in a separate case study. The focus was thus shifted to simulating a mechanical abuse loading condition on the Structural Battery, with an emphasis on the disparity in its response when incorporated within a CF laminate. To accurately forecast and measure internal short circuit and thermal runaway, Mechanical-Electrical-Thermal coupled analyses were essential. Specifically, the mechanical solver was utilized to anticipate internal short circuit based on load reduction or stress/strain threshold, contingent on the chosen failure criteria. Meanwhile, the electric and thermal solvers were employed to calculate voltage decrease and thermal runaway respectively, due to internal short circuit [75]. Based on available literature [76], battery discretization can be executed through three distinct methods in the commercial solver LS-Dyna, as schematically reviewed in Figure 10.

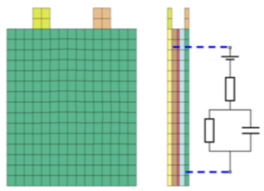
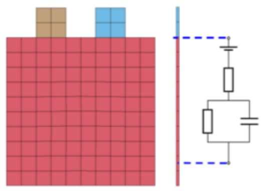
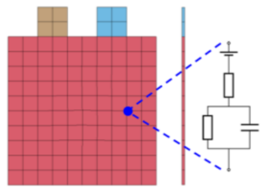
	Solid layer model	Tshell model	Batmac model
			
Keyword	*EM_RANDLESS_SOLID	*EM_RANDLESS_TSHELL	*EM_RANDLESS_BATMAC
Scale	Micro scale	Meso scale	Macro scale
Characteristics	+ Analysis of all layers is possible since meshed with solid elements + Same mesh used for mechanics, thermal and EM – Many elements with large AR and small mechanical time step	+ Beneficial modeling of thin cells + EM and thermal use automatically generated solid mesh + Faster runs (less elements and larger timestep) – Behavior of the layers can not be analyzed in detail	+ One or a few solid elements through the thickness for mechanics, EM and thermal + 2 fields at each node (positive and negative current collectors) + Computationally cheap allowing pack level simulations – Behavior of the layers can not be analyzed

Figure 9 – Battery modeling available approaches within LS-Dyna solver.

For the sake of clarity, the electrochemical behaviour of batteries is described by the Randles (equivalent) circuits that contains an open-circuit voltage, an internal resistance, and a resistance-capacitance pair for polarization and damping effects. This representation is used to capture impedance increase/decrease due to equivalent physical processes. A comprehensive review of the parameters required to correctly define the battery model in LS-Dyna is provided in [76, 77], along with the experimental tests to define the parameters themselves. When a cell is shorted, the Randles circuits in the shorted area are replaced by short circuit resistances. Although these three models share the same physical governing equations, they have different element types, material information and numerical implementation.

In the solid layer model, each individual component of the battery (e.g., negative current collector, electrolyte layer, separator, electrolyte layer, positive current collector) is resolved and represented by one layer of solid elements. Each component may have different thickness and material properties.

A network of Randles circuits connect pairs of nodes in consecutive opposite current collectors. In the tshell model, composite tshell elements with larger thickness are used instead of solid elements. Along the thickness direction, a composite tshell element contains multiple integration points, and each of them corresponds to one individual component. The time saving in the tshell model comes from the mechanical solver that applies the equivalent single layer theory to solve for nodal displacements. The electrical and thermal solvers, on the other hand, rebuild an internal mesh that resolves each individual component and then solve equations on it. The batmac model treats a cell as a homogeneous solid, where large solid elements can be used. With this approach, each node is assumed to contain two electrical potentials connected by one Randles circuit. These two potentials act like electrical potentials in positive and negative current collectors. They are solved separately with electrical conductivities adjusted to account for the difference between the thickness of the cell and current collectors.

In the case study under discussion, since available information involved the mechanical properties of the entire RMS battery cell, without the detail on its layers, it was decided to adopt the batmac model. Furthermore, the inherent approximation within this discretization strategy, which assumes the presence of both electrical potentials at each node, rendered it impossible to account for an ISC triggered by the proximity of the anode and cathode. However, it was feasible to consider an ISC initiated by overcoming a specific strain threshold, which was set to be 90% of the failure strain for the RMS battery material.

Regarding the thermal and electrical properties of the RMS cell, references were drawn from literature, specifically [78, 79]. The relevant properties can be found in Table 2 and 3. For the sake of completeness, Table 2 has been supplemented with the thermal properties both of AS4/8552 carbon fiber and steel, the material used respectively for the laminate and the intruder [80, 81]. Noteworthy is that the information presented in the Tables is based on the assumption that the materials within the RMS battery, for both the current collectors, are isotropic both from thermal and electrical point of view.

Table 2 – Thermal properties for the components involved into the numerical model.

Component	Specific Heat [J/Kg C°]	Thermal Conductivity [W/m K]
Anode Current Collector	385	398
Cathode Current Collector	902	237
Battery Cell	790.9	363.4
Intruder	502.1	16.26
laminate	0.8	1580

Table 3 – Electrical properties for the components involved into the numerical model.

Component	Electrical Conductivity [Ω m]
Anode Current Collector	$2.9*10^{8}$
Cathode Current Collector	$3.3*10^{8}$
Battery Cell	*
Intruder	-
laminate	-

The first simulation taken into account involved the application of mechanical abuse loading on a single RMS battery cell via a hemispherical intruder. The intruder was assigned a predetermined displacement profile, while the RMS battery cell was clamped on the nodes of the face opposite to the one where the impact with the hemispherical intruder took place. The boundary conditions are schematically depicted in Figure 11.

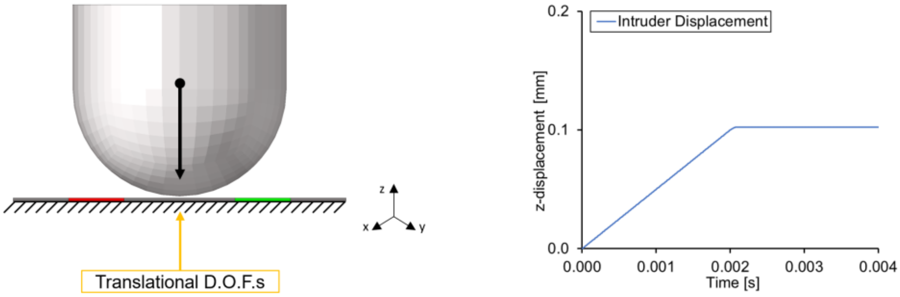


Figure 10 – Boundary conditions adopted for the mechanical abuse loading condition applied on the single RMS battery cell (left) with a focus on the displacement profile assigned to the intruder (right).

The very low displacement was chosen to reduce computational time, compatibly with the time steps of the three solvers, and by positioning the intruder as close to the battery cell as possible. To accurately compare and assess the impact of the RMS cells integration into the CF laminate, an initial numerical campaign was conducted to determine the minimum intruder displacement that would result in a short circuit condition. Subsequently, the velocity was fixed, in accordance with previous research, and the displacement was kept constant from 0.002 seconds onward. For the sake of clarity, the intruder's displacement profile was selected such that it would cease upon reaching the short circuit condition. The preliminary numerical campaign revealed that if the intruder halted just before that threshold, the voltage drop would not occur, as it would not have reached the failure strain level required for a short circuit.
The same boundary conditions were then applied to the laminate with embedded structural batteries, as illustrated in Figure 12. In detail, the same displacement profile for the intruder was maintained, ensuring that the distance between the intruder and the structural battery in the first case was equivalent to the distance between the intruder and the first ply of the laminate in this case. The results of those simulations are schematically presented in Figure 13. The higher contact force obtained in the second case (between the intruder and the first ply of the composite laminate) than in the first case (where the contact force was between the intruder and the structural battery) can be attributed to the fixed displacement of the intruder (treated as a rigid entity) and the disparity in the stiffnesses assigned to the two reference materials for the battery and the laminate. At the same time, while in the first case the voltage drop happens in the same time the contact force reaches its maximum value, in the second case the structural reinforcement of the composite laminate shows its functional contribution in delaying (as in the case of the first structural battery module, the one nearer to the intruder impact region) or even preventing (as in the case of the second structural battery module) short circuit phenomena. The temperature exhibits a slight linear increase, which is attributed to the assumption that the materials are thermally isotropic.

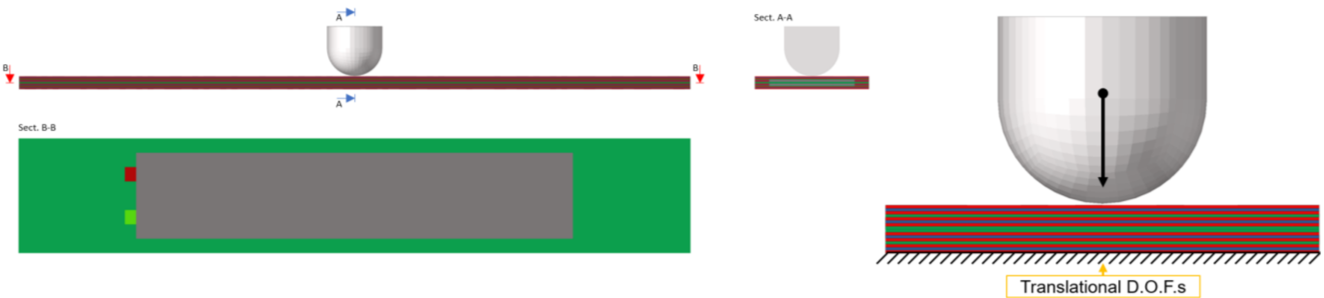


Figure 11 – CF laminate breakdown (left) with a focus on the boundary conditions adopted for the mechanical abuse loading condition simulation (right).

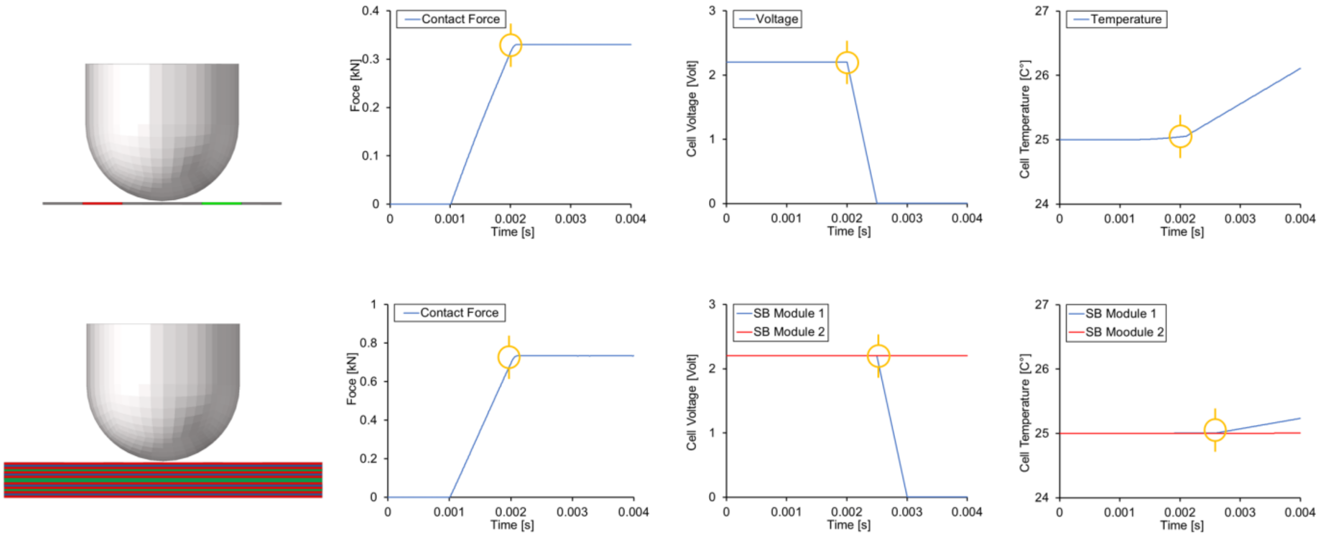


Figure 12 – Mechanical abuse loading condition simulation results: comparison between the single battery cell (top) and the laminate with embedded SBs (bottom). In detail, contact force (left), voltage drop (middle), and temperature arise (right) are compared.

4. Conclusions

The paper highlights the critical role of understanding lithium-ion battery failure mechanisms for ensuring their safe implementation in electric aviation, a key driver for a more sustainable future in the aerospace industry.

The paper emphasizes the importance of multiphysics simulations that couple structural, electrical, and thermal responses during battery design. This holistic approach is crucial for developing inherently safer lithium-ion batteries for demanding aviation applications.

Furthermore, the concept of Structural Batteries emerges as a promising technology for electric air transport. By integrating energy storage and load-bearing functionalities, Structural Batteries offer the potential to reduce weight, a significant constraint in electric aircraft design, ultimately extending range and payload capacity.

The presented analysis underscores the challenges and future directions for structural battery research. Advanced Finite Element Analysis simulations are identified as a pivotal tool for modeling structural battery behavior under various abuse conditions, particularly those leading to internal short circuits, a major safety concern. A numerical simulation of an abuse loading condition on a Structural Battery is shown, emphasizing the variation in its response when integration within a CF laminate is considered. In detail, the findings of these simulations highlight the significant role of the structure in mitigating or even eliminating the risk of short circuit phenomena when the structural battery modules are incorporated into the laminated structure.

By leveraging the predictive capabilities of these simulations, researchers can accelerate the development of safer and more efficient structural batteries, paving the way for the widespread adoption of electric aviation and a more sustainable future for air travel.

5. Contact Author Email Address

gennaro.dimauro@unina.it (corresponding author)
michele.guida@unina.it
luismanuel@niar.wichita.edu
gerardo.olivares@wichita.edu

6. Copyright Statement

References

[1] Goodenough J B. Energy storage materials: a perspective. *Energy storage materials*, Vol. 1, pp 158-161, 2015.

[2] Shan X Y, Li F, Wang D W, Cheng H M. The smart era of electrochemical energy storage devices. *Energy Storage Materials*, Vol. 3, pp 66-68, 2016.

[3] Yan J, Li K, Chen H, Wang Q, Sun J. Experimental study on the application of phase change material in the dynamic cycling of battery pack system. *Energy Conversion and Management*, Vol. 128, pp 12-19, 2016.

[4] Yan J, Wang Q, Li K, Sun J. Numerical study on the thermal performance of a composite board in battery thermal management system. *Applied Thermal Engineering*, Vol. 106, pp 131-140, 2016.

[5] Li N, Chen Z, Ren W, Li F, Cheng H M. Flexible graphene-based lithium-ion batteries with ultrafast charge and discharge rates. *Proc. of the National Academy of Sciences*, Vol. 43, 109, pp 17360-17365, 2012.

[6] Jeong G, Kim Y U, Kim H, Kim Y J, Sohn H J. Prospective materials and applications for Li secondary batteries. *Energy & Environmental Science*, Vol. 6, 4, pp 1986-2002, 2011.

[7] Doughty D H, Roth E P. A general discussion of Li ion battery safety. *The Electrochemical Society Interface*, Vol. 2, 21, pp 37, 2012.

[8] Wang Q, Mao B, Stoliarov S I, Sun J. A review of lithium-ion battery failure mechanisms and fire prevention strategies. *Progress in Energy and Combustion Science*, Vol. 73, pp 95-131, 2019.

[9] Larsson F, Andersson P, Blomqvist P, Lorén A, Mellander B E. Characteristics of lithium-ion batteries during fire tests. *Journal of Power Sources,* Vol. 271, pp 414-420, 2014.

[10]Fernandes Y, Bry A, De Persis S. Identification and quantification of gases emitted during abuse tests by overcharge of a commercial Li-ion battery. *Journal of power sources*, Vol. 389, pp 106-119, 2018.

[11]Lamb J, Orendorff C J, Amine K, Krumdick G, Zhang Z, Zhang L, Gozdz A S. Thermal and overcharge abuse analysis of a redox shuttle for overcharge protection of LiFePO4. *Journal of power sources*, Vol. 247, pp 1011-1017, 2014.

[12]Ohsaki T, Kishi T, Kuboki T, Takami N, Shimura N, Sato Y, Satoh A. Overcharge reaction of lithium-ion batteries. *Journal of power sources*, Vol. 1-2, 146, pp 97-100, 2005.

[13]Ouyang M, Ren D, Lu L, Li J, Feng X, Han X, Liu G. Overcharge-induced capacity fading analysis for large format lithium-ion batteries with LiyNi1/3Co1/3Mn1/3O2+ LiyMn2O4 composite cathode. *Journal of power sources*, Vol. 279, pp 626-635, 2015.

[14]Park Y, Kim N H, Cho S B, Kim J M, Kim G C, Kim M S, Jung Y M. Characterization of the passivating layer on Li [Ni0. 31Co0. 32Mn0. 28Al0. 09] O2 cathode in the overcharge state. *Journal of Molecular Structure*, Vol. 1-3, 974, pp 139-143, 2010.

[15]Ye J, Chen H, Wang Q, Huang P, Sun J, Lo S. Thermal behavior and failure mechanism of lithium-ion cells during overcharge under adiabatic conditions. *Applied energy*, Vol. 182, pp 464-474, 2015.

[16]Yuan Q, Zhao F, Wang W, Zhao Y, Liang Z, Yan D. Overcharge failure investigation of lithium-ion batteries. *Electrochimica Acta*, Vol. 178, pp 682-688, 2015.

[17]Lai X, Zheng Y, Zhou L, Gao W. Electrical behavior of overdischarge-induced internal short circuit in lithium-ion cells. *Electrochimica Acta*, Vol. 278, pp 245-254, 2015.

[18]Abaza A, Ferrari S, Wong H K, Lyness C, Moore A, Weaving J, Bhagat R. Experimental study of internal and external short circuits of commercial automotive pouch lithium-ion cells. *Journal of Energy Storage*, Vol. 16, pp 211-217, 2018.

[19]Dubaniewicz Jr T H, DuCarme J P. Further study of the intrinsic safety of internally shorted lithium and lithium-ion cells within methane-air. *Journal of loss prevention in the process industries*, Vol. 32, pp 165-173, 2014.

[20]Spotnitz R, Franklin J. Abuse behavior of high-power, lithium-ion cells. *Journal of power sources*, Vol. 1, 113, pp 81-100, 2003.

[21]Mao B, Chen H, Cui Z, Wu T, Wang Q. Failure mechanism of the lithium-ion battery during nail penetration. *International Journal of Heat and Mass Transfer*, Vol. 122, pp 1103-1115, 2018.

[22]Zhang C, Santhanagopalan S, Sprague M A, Pesaran A A. A representative-sandwich model for simultaneously coupled mechanical-electrical-thermal simulation of a lithium-ion cell under quasi-static indentation tests. *Journal of Power Sources*, Vol. 298, pp 309-321, 2015.

[23]Sahraei E, Meier J, Wierzbicki T. Characterizing and modeling mechanical properties and onset of short circuit for three types of lithium-ion pouch cells. *Journal of Power Sources*, Vol. 247, pp 503-516, 2014.

[24]Sahraei E, Kahn M, Meier J, Wierzbicki T. Modelling of cracks developed in lithium-ion cells under mechanical loading. *Rsc Advances*, Vol. 98, 5, pp 80369-80380, 2015.

[25]Greve L, Fehrenbach C. Mechanical testing and macro-mechanical finite element simulation of the deformation, fracture, and short circuit initiation of cylindrical Lithium-ion battery cells. *Journal of Power Sources*, Vol. 214, pp 377-385, 2012.

[26]Sahraei E, Hill R, Wierzbicki T. Calibration and finite element simulation of pouch lithium-ion batteries for mechanical integrity. *Journal of Power Sources*, Vol. 201, pp 307-321, 2012.

[27]Wierzbicki T, Sahraei E. Homogenized mechanical properties for the jellyroll of cylindrical Lithium-ion cells. *Journal of power sources*, Vol. 241, pp 467-476, 2013.

[28]Sahraei E, Campbell J, Wierzbicki T. Modeling and short circuit detection of 18650 Li-ion cells under mechanical abuse conditions. *Journal of Power Sources*, Vol. 220, pp 360-372, 2012.

[29]Sheidaei A, Xiao X, Huang X, Hitt J. Mechanical behavior of a battery separator in electrolyte solutions. Journal of Power Sources, Vol. 20, 196, pp 8728-8734, 2011.

[30]Cannarella J, Liu X, Leng C Z, Sinko P D, Gor G Y, Arnold C B. Mechanical properties of a battery separator under compression and tension. *Journal of the Electrochemical Society*, Vol. 11, 161, pp F3117, 2014.

[31]Gor G Y, Cannarella J, Prévost J H, Arnold C B. A model for the behavior of battery separators in compression at different strain/charge rates. *Journal of The Electrochemical Society*, Vol. 11, 161, pp F3065, 2014.

[32]Lai W J, Ali M Y, Pan J. Mechanical behavior of representative volume elements of lithium-ion battery cells under compressive loading conditions. *Journal of Power Sources*, Vol. 245, pp 609-623, 2014.

[33]Lai W J, Ali M Y, Pan J. Mechanical behavior of representative volume elements of lithium-ion battery modules under various loading conditions. *Journal of Power Sources*, Vol. 248, pp 789-808, 2014.

[34]Ali M Y, Lai W J, Pan J. Computational models for simulations of lithium-ion battery cells under constrained compression tests. *Journal of Power Sources*, Vol. 242, pp 325-340, 2013.

[35]Avdeev I, Gilaki M. Structural analysis and experimental characterization of cylindrical lithium-ion battery cells subject to lateral impact. *Journal of Power Sources*, Vol. 271, pp 382-391, 2014.

[36]Wang W, Yang S, Sun F, Yu Q. The clay-like mechanics model of cylindrical lithium-ion battery cells under radial compression. *Energy Procedia*, Vol. 88, pp 652-655, 2016.

[37]Xu J, Liu B, Wang L, Shang S. Dynamic mechanical integrity of cylindrical lithium-ion battery cell upon crushing. *Engineering Failure Analysis*, Vol. 53, pp 97-110, 2015.

[38]Xu J, Liu B, Hu D. State of charge dependent mechanical integrity behavior of 18650 lithium-ion batteries. *Scientific reports*, Vol. 1, 6, pp 21829, 2016.

[39]Xu J, Liu B, Wang X, Hu D. Computational model of 18650 lithium-ion battery with coupled strain rate and SOC dependencies. *Applied Energy*, Vol. 172, pp 180-189, 2016.

[40]Liu B, Yin S, Xu J. Integrated computation model of lithium-ion battery subject to nail penetration. *Applied energy*, Vol. 183, pp 278-289, 2016.

[41]Maleki H, Howard, J N. Internal short circuit in Li-ion cells. *Journal of Power Sources*, Vol 2, 191, pp 568-574, 2009.

[42]Cai W, Wang H, Maleki H, Howard J, Lara-Curzio E. Experimental simulation of internal short circuit in

Li-ion and Li-ion-polymer cells. *Journal of Power Sources*, Vol. 18, 196, pp 7779-7783, 2011.

[43]Doughty D H. Vehicle battery safety roadmap guidance (No. NREL/SR-5400-54404). National Renewable Energy Lab. (NREL), Golden, CO (United States), 2012.

[44]Hatchard T D, Trussler S, Dahn J R. Building a “smart nail” for penetration tests on Li-ion cells. *Journal of Power Sources*, Vol. 247, pp 821-823, 2014.

[45]Lamb J, Orendorff C J. Evaluation of mechanical abuse techniques in lithium-ion batteries. *Journal of Power Sources*, Vol. 247, pp 189-196, 2014.

[46]Lamb J, Orendorff C J, Steele L A M, Spangler S W. Failure propagation in multi-cell lithium-ion batteries. *Journal of Power Sources*, Vol. 283, pp 517-523, 2015.

[47]Feng X, Sun J, Ouyang M, Wang F, He X, Lu L, Peng H. Characterization of penetration induced thermal runaway propagation process within a large format lithium-ion battery module. *Journal of Power Sources*, Vol. 275, pp 261-273, 2015.

[48]Zhao R, Liu J, Gu J. Simulation and experimental study on lithium-ion battery short circuit. *Applied Energy*, Vol. 173, pp 29-39, 2016.

[49]Xia Y, Wierzbicki T, Sahraei E, Zhang X. Damage of cells and battery packs due to ground impact. *Journal of Power Sources*, Vol. 267, pp 78-97, 2014.

[50]Ozawa K. Lithium-ion rechargeable batteries: materials, technology, and new applications. *John Wiley & Sons*, 2012.

[51]Pistoia G. Electric and hybrid vehicles: Power sources, models, sustainability, infrastructure and the market. *Elsevier*, 2010.

[52]Yildiz M. Initial airworthiness requirements for aircraft electric propulsion. *Aircraft engineering and aerospace technology*, Vol. 8, 94, pp 1357-1365, 2022.

[53]Adam T J, Liao G, Petersen J, Geier S, Finke B, Wierach P, Wiedemann M. Multifunctional composites for future energy storage in aerospace structures. *Energies*, Vol. 2, 11, pp 335, 2018.

[54]Schutzeichel M O H, Kletschkowski T, Linde P, Asp L E. Experimental characterization of multifunctional polymer electrolyte coated carbon fibres. *Functional Composites and Structures*, Vol. 2, 1, pp 025001, 2019.

[55]Schutzeichel M O H, Kletschkowski T, Linde P, Asp L E. Experimental characterization of multifunctional polymer electrolyte coated carbon fibres. *Functional Composites and Structures*, Vol. 2, 1, pp 025001, 2019.

[56]Shirshova N, Bismarck A, Carreyette S, Fontana Q P, Greenhalgh E S, Jacobsson P, Wienrich M. Structural supercapacitor electrolytes based on bicontinuous ionic liquid–epoxy resin systems. *Journal of Materials Chemistry A*, Vol. 48, 1, pp 15300-15309, 2013.

[57]Scholz A E, Hermanutz A, Hornung M. Feasibility analysis and comparative assessment of structural power technology in all-electric composite aircraft. *Proc. of 67. Deutscher Luft-und Raumfahrtkongress*, 2018.

[58]Karadotcheva E, Nguyen S N, Greenhalgh E S, Shaffer M S P, Kucernak A R J, Linde P. Structural Power Performance Targets for Future Electric Aircraft. Energies, Vol. 14, pp 6006, 2021.

[59]Nguyen S N, Millereux A, Pouyat A, Greenhalgh E S, Shaffer M S, Kucernak A R, Linde P. Conceptual multifunctional design, feasibility and requirements for structural power in aircraft cabins. *Journal of Aircraft*, Vol. 3, 58, pp 677-687, 2021.

[60]Riboldi C E, Trainelli L, Biondani F. Structural batteries in aviation: A preliminary sizing methodology. *Journal of Aerospace Engineering*, Vol. 4, 33, pp 04020031, 2020.

[61]Ihrner N, Johannisson W, Sieland F, Zenkert D, Johansson M. Structural lithium-ion battery electrolytes via reaction induced phase-separation. *Journal of Materials Chemistry A*, Vol 48, 5, pp 25652-25659, 2017.

[62]Johannisson W, Ihrner N, Zenkert D, Johansson M, Carlstedt D, Asp L E, Sieland F. Multifunctional performance of a carbon fiber UD lamina electrode for structural batteries. *Composites Science and Technology*, Vol. 168, pp 81-87, 2018.

[63]Javaid A, Ali M Z. Multifunctional structural lithium-ion batteries for electrical energy storage applications.

Materials Research Express, Vol. 5, 5, pp 055701, 2018.

[64]Johannisson W, Zenkert D, Lindbergh G. Model of a structural battery and its potential for system level mass savings. *Multifunctional Materials*, Vol. 3, 2, 035002, 2019.

[65]Laurin F, Mavel A, Saffar F, Beutl A, Kühnelt H. Experimental and numerical evaluation of residual mechanical performance of carbon/epoxy laminated coupons after integration of solid battery cells for aeronautical applications. *Composites Science and Technology*, Vol. 247, pp 110384, 2024.

[66]Kühnelt H, Beutl A, Mastropierro F, Laurin F, Willrodt S, Bismarck A, Romano F. Structural batteries for aeronautic applications—state of the art, research gaps and technology development needs. *Aerospace*, Vol. 1, 9, pp 7, 2021.

[67]Di Mauro G, Guida M, Olivares G, Gomez L M. Paving the Way for the Electrified Future of Flight: Safety Criteria Development for Integrating Structural Batteries in Aircraft. *Aerotecnica Missili & Spazio*, pp 1-7, 2024.

[68]Asp L E, Bouton K, Carlstedt D, Duan S, Harnden R, Johannisson W, Zenkert D. A structural battery and its multifunctional performance. *Advanced Energy and Sustainability Research*, Vol. 3, 2, pp 2000093, 2021.

[69]Yücel Y D, Zenkert D, Lindström R W, Lindbergh G. LiFePO4-coated carbon fibers as positive electrodes in structural batteries: Insights from spray coating technique. *Electrochemistry Communications*, Vol. 160, pp 107670, 2024.

[70]Yücel Y D, Bouton K, Adolfsson E, Dykhoff H, Pettersson J, Trey S, Lindbergh G. Structural Batteries with LiFePO4-Impregnated Carbon Fibers, 2024.

[71]Laurin F, Beutl A, Jiang Q, Kühnelt H. (2023, June). Concepts for integrating electrical energy storage into CFRP laminate structures for aeronautic applications. *Proc. of Journal of Physics: Conference Series*, Vol. 2526, 1, pp 012062, 2023.

[72]Baluch A H, Falcó O, Jiménez J L, Tijs B H, Lopes C S. An efficient numerical approach to the prediction of laminate tolerance to Barely Visible Impact Damage. *Composite Structures*, Vol. 225, pp 111017, 2019.

[73]Falcó O, Ávila R L, Tijs B, Lopes C S. Modelling and simulation methodology for unidirectional composite laminates in a Virtual Test Lab framework. *Composite Structures*, Vol. 190, pp 137-159, 2018.

[74]Garstka T, Ersoy N, Potter K D, Wisnom M R. In situ measurements of through-the-thickness strains during processing of AS4/8552 composite. *Composites Part A: applied science and manufacturing*, Vol. 12, 38, pp 2517-2526, 2007.

[75]Moon J, Chang H, Lee J, Kim C W. Prediction of Internal Circuit and Mechanical-Electrical-Thermal Response of Lithium-Ion Battery Cell with Mechanical-Thermal Coupled Analysis. *Energies*, Vol. 3, 15, pp 929, 2022.

[76]Bateau-Meyer S, L'Eplattenier P, Deng J, Zhu M, Bae C, Miller T. Randles circuit parameters set up for battery simulations in LS-DYNA. In *Proceedings of 15th International LS-DYNA Users Conference*, 2018.

[77]LS-DYNA Manual Volume II R13.

[78]Wei L, Lu Z, Cao F, Zhang L, Yang X, Yu X, Jin L. A comprehensive study on thermal conductivity of the lithium-ion battery. *International Journal of Energy Research*, Vol. 12, 44, pp 9466-9478, 2020.

[79]Tsakiris V, Kappel W, Alecu G. Solid state diffusion welding of Cu-Fe/Al/Ag and Al-Ni dissimilar metals. *Journal of Optoelectronics and Advanced Materials*, Vol. 9, 13, pp 1176, 2011.

[80]Yafei S, Yongjun T, Jing S, Dongjie N. Effect of temperature and composition on thermal properties of carbon steel. In *Chinese Control and Decision Conference,* IEEE, pp. 3756-3760, 2009.

[81]Scott E P, Beck J V. Estimation of thermal properties in epoxy matrix/carbon fiber composite materials. *Journal of composite materials*, Vol. 1, 26, pp 132-149, 1992.