Heat Transfer and Cell Failure Analysis for Configuration of a Non-Propagating Li-ion Battery Pack with a Copper Microfibrous Cooling Structure during Extreme-Condition Pulsed Power Operation

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Abstract

IntraMicron is building a high-power 1000V battery system for NSWC Philadelphia Code 32 to provide additional energy storage capacity for the support of future weapons and other shipboard systems. The modules and system are being designed to mitigate cell-to-cell and module-to-module propagation failure events under harsh operating conditions. This work focuses on the simulated thermal performance of each 50V 12S module under normal operation and cell-failure scenarios. A thermal model for the Li-ion battery pack based on COMSOL Multiphysics has been established to simulate the heat transfer process inside the battery power system for regulating cell temperature during 4C/15C power cycles. Multiple cell configurations of the 12S module were assessed for performance and manufacturability. To fully gauge the capabilities of the cooling structure, it is important to understand the effect of one-cell thermal failure on the nearby Li-ion cells during an unexpected extreme heat generation event. The 2D failure results for 3×4 offset configuration reveal that the maximum cell surface temperature was obtained as ca. 53.1°C for the cells adjacent to the failed cell, indicating that the enhanced cooling structure removes and dissipates sufficient heat to prevent cascade failure. A 3D model structure was also developed to simulate the failure event through coupling of heat transfer, fluid flow, and solid mechanics submodels. To augment the safety assessment of the module during normal operation and single-cell failure, the initial pressure profile inside the cell, the surface temperature at the cell's safety vent, and the total displacement and stress profiles of the cell's top cover were considered through the fluid-structure interaction with the solid mechanics physics package.

Keywords

Metal microfibrous media; hybrid heat transfer modeling; high-power battery pack; Li-ion cell failure and structure safety; energy storage and conversion.

Introduction

A well-designed battery thermal management system (BTMS) is crucial to maintain a Li-ion battery pack's temperature within an acceptable range and uniformity. Initially, passive thermal management (PTM) was achieved using solid-liquid phase-change material (PCM) on the Li-ion battery pack [1]. However, for high peak or pulsed power operating conditions, active thermal management (ATM) is necessary for its higher heat transfer capability and removal rate to dissipate the large amounts of heat generated inside neighboring cells. Liquid cooling enables high-power acceleration in some existing EVs/HEVs such as the Chevrolet and Tesla Model S [2]. Fathabadi used PCM/expanded graphite composite with air duct cooling flow through the battery pack to achieve improved performance [3]. Recently, active cooling tubes were inserted and sintered together with a porous metal microfibrous media structure (MFM) fully embedded with PCM waxes to overcome the low thermal conductivity limitations of paraffin [4]. During load cycling, mechanical cell failure may occur due to cell plasticity deformation caused by compression or tension in the BTMS and cooling structure [5]. Moreover, battery failure or thermal runaway usually occurs when the cell temperature exceeds a certain threshold, resulting in subsequent heat-producing decomposition processes that further increase the cell temperature. This paper establishes a thermal model to evaluate a 12S Li-ion battery pack's performance, comparing the cell surface temperature differences for 2x6 and 3x4 12S configurations. A safety evaluation on the cell structure is also conducted by modeling burst disc stress and displacement with a structural mechanics inclusion.

Model Structure with Structural Mechanics

The COMSOL Multiphysics platform, along with a heat transfer module, was selected for simulating the heat transfer process in a 12S Li-ion battery pack. The 3D simulation was completed by constructing a physical model of the system and coupling it with a heat transfer model in the battery pack including fluid flow in the cooling tubes. A simplified 2D model structure was used to facilitate the module design and module structure evaluation process because of its drastically reduced computational time. The 50 V modules consist of twelve 30 Ah Li-ion cells connected in series, and they were simulated through 4C/15C charge/discharge cycles using previously validated model parameters. The Li-ion cells were assumed to be packed in the actively cooled MFM-PCM cooling structure and operated at an ambient temperature of 60°C. Depending on the specific application, the metal MFM structure can be customized to achieve a specific void volume and heat transfer performance. The enhanced heat transfer of MFM enables nearly instantaneous access to the latent heat capacity of the PCM when responding to temperature changes from dynamic high-power loads. The active cooling tube is an essential component for the MFM-PCM battery thermal management system during extreme-condition high-power cycles. The cooling tube is embedded inside the MFM-PCM matrix and is able to efficiently transfer heat which was absorbed and stored in the MFM-PCM matrix as well as removing cell-generated heat from the surface of the cells. The unique design for the active-cooling structure allows the MFM-PCM matrix to normalize the Li-ion cell surface temperatures in the pack during frequent charge/discharge cycles at high discharge rates. Another advantage is that the specific design enables the battery pack to function at an ambient temperature above the melting point of the paraffin wax.

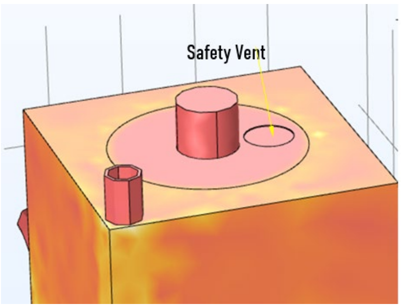


Figure 1. Geometric structure for the Li-ion cell packed inside the MFM-PCM block matrix embedded with the cooling tube.

In this study, the battery pack model and simulation were applied to a group of 30 Ah Li-ion cells with high pulsed power capability. The cells have a diameter of 54 mm, a height of 222 mm, a weight of 1100 g, and a volume of 0.51 dm^3. The battery was cycled between 40°C and 50°C at a 4C charge rate and 15C discharge rate and operated from 91.7% SoC to 100% DoD for testing and evaluation of the structure's thermal performance. The Li-ion cells use a graphite-based anode and nickel oxide-based cathode, and the electrolyte is a blend of LiPF6 and carbonate solvents. To test and evaluate the high-power battery packs, an Arbin battery tester capable of operating at a discharge current up to 600 A was used. The prototypical MFM-PCM matrix structure with active liquid-cooling enhancement was described in previous publications [6]. The structure model parameters for the battery pack were adopted from simulation and validation testing in a similar study with 12 cells in series (12S). Details of this data are not shown because of its proprietary nature. Key parameters were used to determine a practical model and simulation solution. Additionally, theoretical simulation of cascade catastrophic failure for a battery pack can be performed with this model to evaluate extreme condition battery operation.

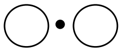
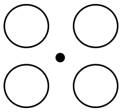
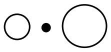
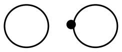
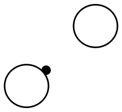
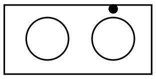
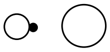
For the cell failure modeling via the COMSOL-6 platform, the heat transfer and the structural mechanics modules were selected. Two heat transfer submodels (HT1+HT2) were constructed for multiphysics coupling to separate the two fluids in the cell gas and wax fluid. The fluid submodel (Fluid1) was coupled with HT1 to include the cell gas fluid, which was then coupled with the structural mechanics (Mech1) to evaluate the structural interaction between the cell gas fluid, the burst disc, and the cell can. This was especially important at the top cover area. The model evaluated the cell internal pressure, cell surface temperature, and the cell safety vent temperature for a single Cell (number 12) in the MFM-PCM structure near the water outlet after the cell failure via one-second energy release of 511.6 kJ. The coolant temperature was set to 38.18°C, and the ambient temperature was set to 59.04°C. For the MFM-PCM structure, the following parameters were defined: a thermal conductivity correction factor of 0.483, a thin film wrap thermal conductivity 0.15 W/m-K, an inner cooling tube heat transfer coefficient of 3925 W/m^2-K, and an external wall heat transfer coefficient of 5 W/m^2-K. The internal cell pressure can be expressed through the initial gas and DMC saturated vapor pressure [7]. The applied pressure in the cell headspace reached approximately 400 kPa during the initial tests for structure safety evaluation.

The safety vent burst disc was assumed to be a grooved thinner metal foil in the cell top cover for the structural mechanics interaction. The model structure was coupled with two heat transfer submodels, one gas fluid flow submodel, and the solid mechanics submodel. The cell can and the top cover wall were defined as low carbon steel with a shell thickness of 0.04 inches. The groove depth of the vent had a thickness of 0.01 inches. Cell failure was defined to occur with a one-second heat release that started at 7586.74 seconds. The simulation used the time-dependent solver via four segregated solution steps.

Simulation Results

For the 2D cycling tests, it was assumed that a thin thermal resistive layer with a thickness of 0.01 mm exists between the cell and the plastic insulating wrap and the equivalent heat transfer coefficient at the interface was thus obtained as 1775 W/m^2-K. The paraffin wax has with a melting point of 54.8°C. Thus, the estimated thermal conductivity of 58 W/m-K was applied to the cooling structure to evaluate different designs and optimized configurations. The cells connected in series were assumed to be operated at 4C/15C charge/discharge cycles. Four pack-cooling configurations were evaluated with the 2D COMSOL-4.3 thermal model to simulate the high-rate charge/discharge cycles, and the results are shown in Table 1. For each structure, except Type-IV, the 12 cells were arranged in either a 2x6 or 3x4 pattern in the structure. The Type-IV pack contains 14 cells in a 5-4-5 configuration. The results show that the temperatures for the Type-II pack are slightly higher than the other three MFM-PCM cooling structure designs. The highest cell surface temperature is 47.9°C near an adjacent cell using the 2D simulation method. The model results show that there is a small temperature difference on the cell surfaces for the Type-I, III and IV designs. The 2D simulation results show that all four types of battery packs, using the initial MFM-PCM design configurations with active cooling loops, are able to satisfy the BTMS requirement for direct heat removal during short charge/discharge high-power cycles.

Table 1. Simulated steady peak temperature after the 5th cycle at t=4700 s.

Domain Point Probe Location	I. 2x6 OFFSET	II. 3x4 SYMMETRIC	III. 3x4 OFFSET	IV. 545 OVERSIZE
On the block, between 2 cells 	46.5°C	47.2°C	46.6°C	46.5°C
On the block, between 4 cells 	43.7°C	46.1°C	43.8°C	43.9°C
Between a cell and cooling tube 	45.1°C	43.6°C	45.2°C	45.3°C
At cell surface, near another cell 	47.0°C	47.9°C	46.8°C	46.7°C
At cell surface, diagonal to another cell 	46.9°C	47.1°C	47.0°C	46.1°C
Block edge 	44.8°C	44.7°C	44.8°C	43.9°C
Cooling Tube Edge 	43.7°C	43.5°C	43.8°C	44.0°C

Failure Analysis

Power system reliability and operating safety are significant challenges for the application of Li-ion battery packs in various fields due to concerns regarding heat generation, overheating, and thermal runaway. This is particularly problematic because the discharge process of a Li-ion cell generates a large amount of heat, particularly during short high-power cycles in cylindrical cells. The use of active cooling loops, however, enables rapid heat removal during high-power short cycles and maintains a cooler and safer operating environment for the MFM-PCM block. As a result, the unique design of the cooling system effectively reduces the risk of overheating in the Li-ion power system. Nevertheless, it is essential to consider the durability of the MFM-PCM cooling block in the event of thermal runaway or unexpected cell failure in the battery pack.

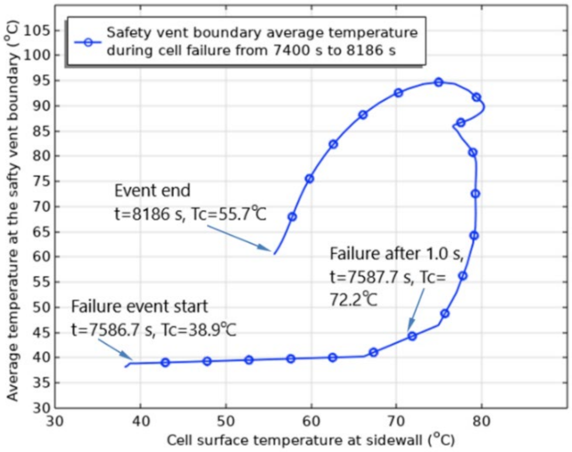


Figure 2. Simulated average temperature at the safety vent as a function of the cell surface temperature at the sidewall.

The ability of the actively cooled MFM-PCM pack to mitigate cascade failure was assessed by evaluating the simulated thermal response in the event of a single-cell failure. The battery pack was assumed to be operating normally from the first to the sixth cycle until it was fully charged during the seventh cycle. At this point, it was assumed that one of the cells, which was in one of the hottest locations, would unexpectedly fail in one second with a maximum energy release of 511.6 kJ after the seventh cycle charge. This was the total energy of a fully charged 30 Ah Li-ion cell with an additional 33% energy generated from related chemical reactions. The battery pack was still operating in a 60°C ambient environment. During the one-second failure period, the other cells continued regular discharge and then turned off 10 minutes after the single-cell failure. Using this assumption, temperature values are obtained at various locations via thermal modeling computation. For the cells adjacent to the failed cell in the Type-II 3x4 battery pack configuration, the maximum cell surface temperature is approximately 53.3°C. After the failure, the block temperatures between two neighboring cells for all four types of cell configurations approach the wax melting point. The temperatures at the failed cell surface exceed the operating limitation of 60°C. The simulation results show that the thermal failure of one cell in the MFM-PCM structure has no destructive effects on the adjacent cells due to latent heat protection from wax liquefaction and rapid heat removal through active cooling circulation inherent to the unique thermal management design for heat transfer enhancement.

To better understand the effect of cell failure on the battery power system, particularly the structural safety of the cell in the MFM-PCM block, a 3D model was developed with the inclusion of the structural mechanics module. The initial simulation results are reported concerning the cell surface temperature, safety vent temperature, total displacement of the safety vent, and von Mises stress on the safety vent of the top cover. The simulation results show visible differences between the cell sidewall surface and the cell safety vent, as shown in Figure 2. The burst disc temperature for the safety vent increases rapidly at 7587.7 s after the cell failure event, reaching a maximum point of 95°C at the burst disc while the cell surface temperature drops from 80°C to 75°C due to the active cooling through tube circulation. The rapid temperature increase is likely caused by the partial pressure increase from the saturated vapor due to the DMC boiling point near 90°C. The vaporization process through the gas fluid flow enhances heat transfer inside the cell. The displacement on the top cover is a function of the cell internal pressure due to cell failure with the assumed extreme heat generation resulting from the cell decomposition and chemical exothermic reactions inside the Li-ion cell. The maximum displacement obtained is approximately 7.9 μm at 308 kPa after the failure event.

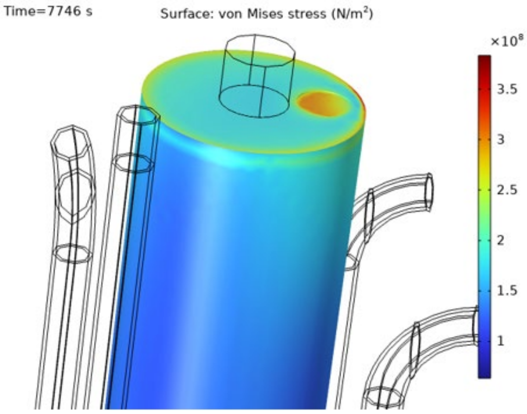


Figure 3. Modeling results for von Mises stress at the safety vent boundary after the cell failure event with extreme heat.

The simulation results for the first principal stress and von Mises stress were obtained to understand the effect of cell failure caused by extreme heat release inside the Li-ion cell on the structural safety of the MFM-PCM block. The first principal stress is the real stress associated with the maximum tensile stress, which is determined by the amount of pressure loading and is normal to the plane where the shear stress is zero. The maximum result for the first principal stress is found to be around 5×10^7 N/m^2 near the cell can edges. The von Mises stress, which predicts the potential failure of a ductile material, was calculated for the top cover with an assumption of fixed constraints for the cell can wall attached to the MFM/PCM block structure. The maximum von Mises stress is found to be around 3.0×10^8 N/m^2 at the cell safety vent boundary, as shown in Figure 3. Although the COMSOL-6 multiphysics platform is capable of coupling different submodels and also can provide better solution routes, the simulation parameters must be refined for changes in pack structure and to provide correlation with actual experimental data. Future work will aim to gain a deeper understanding of Li-ion cell fundamentals during rapid failure events and the performance of the pack structure during these failures with a focus on evaluating for non-propagation. This includes investigating changes in cell gas components and constituents during extreme heat generation within a short period. The results of the future work will enable the proper assessment of cell failure and structure endurance to evaluate the safety of a design prior to real-world failure testing.

Summary

The thermal model developed for the actively cooled MFM-PCM matrix demonstrates the structure can be used to maintain high-power Li-ion cells at an acceptable operating temperature during short charge/discharge cycles under extreme conditions (60°C ambient temperature). The 2D simulation results demonstrate that the neighboring cell surface temperature does not exceed 47.9°C during high-rate normal cycles (4C/15C) for four types of liquid-cooling configuration designs. The single-cell failure models also indicate that the maximum temperature at the cell surface adjacent to the failure cell does not exceed 53.3°C. This suggests that the structure will prevent cell-to-cell propagation due to a thermal excursion. Additionally, the 3D simulation coupled with the structural mechanics module provides valuable information such as cell surface and burst disc temperatures, displacement of the safety vent due to the boundary pressure load and temperature surge, and von Mises stress on the vent structure. Overall, the unique cooling structure of the MFM-PCM matrix enables efficient heat removal from the Li-ion battery pack for high-power operating devices.

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