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**BALLISTIC SIMULATION METHOD FOR LITHIUM-ION BATTERIES
USING THICK SHELL COMPOSITES IN LS-DYNA**

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ABSTRACT

Lithium-ion (Li-ion) batteries have become an important energy storage solution for a wide range of applications from consumer electronics to automobiles. In particular, the automotive industry's push for improved fuel efficiency has led to the development of electric and hybrid-electric vehicles, many of which use Li-ion batteries. In addition to these fuel-saving motivations for Li-ion batteries, the US Army has its own unique mission requirements for onboard energy storage and available power, which could potentially be addressed at least in part, by Li-ion batteries. However, military ground vehicles are also subject to harsh operating conditions and abuse conditions that can cause failures of onboard equipment. Due to complex nature of the batteries, it is numerically challenging to capture the behavior of these batteries under abuse conditions such as a high-energy impact event. Each battery cell is made up of several layers and sub-layers of different materials. If a finite element model is created by meshing each sub-layer with sufficient detail to perform a ballistic simulation, even a single battery cell will have millions of degrees of freedom (DOF). In a hybrid-electric vehicle battery there are typically tens of cells in a module and hundreds of cells in a full pack. Therefore, the computational challenge associated with using finite element analysis (FEA) for ballistic simulations becomes daunting. In this work, a new method is proposed that employs a Thick Shell Composite (TSC) representation of Li-ion batteries using the commercially available FEA software, LS-DYNA. This approach shows promise for modeling the battery at the module or full-pack level with significantly reduced computational cost compared to a more traditional modeling approach. Individual layers are embedded into this TSC in order to reduce the number of finite elements in each cell significantly. Several of these cells are then assembled either in series or parallel to represent the module and the full battery pack. The TSC numerical model is validated by running a simulation of a bullet impact test and comparing the results to the equivalent physical test. The TSC model predictions show good agreement with the experimental results. In addition, three different impact angle scenarios (oblique, vertical, and horizontal) are simulated for one module of a generic Li-ion battery using the new approach. The extent of the predicted battery damage due to these different impact loading conditions are compared both qualitatively and quantitatively.

INTRODUCTION

In July 2011, the Advanced Vehicle Power and Technology alliance (AVPTA) was announced as a partnership between U.S. Department of Energy (DOE) and the U.S. Army to develop new technologies for both commercial and military ground vehicles that will help address top priorities such as decreasing petroleum dependence, increasing ground vehicle fuel efficiency, and enhancing nation's energy security infrastructure. The US Army Tank Automotive Research, Development and Engineering Center (TARDEC) and the DOE Vehicle

Technology Office (VTO) are collaborating as part of this partnership. One area of collaboration is the development of computational modeling and simulation (M&S) and design tools in the Computer Aided Engineering of Batteries (CAEBAT) program.

An important overall goal of CAEBAT is to advance the state of the art physics-based simulation tools for predicting the battery response in order to accelerate fielding safe and robust lithium-ion (Li-ion) batteries [1] that are suitable for use in both commercial and military vehicles with high

onboard electrical power demands. One of the specific objectives is to accelerate the comparative analysis of alternative Li-ion battery designs as drop-in replacements to lead acid 6T batteries. Another objective is to modify and extend the CAEBAT battery simulation tools to predict the response of Li-ion battery modules under abuse conditions experienced in military applications, including high-energy impact events such as bullet strikes.

The focus of this study is to develop finite element models and associated simulation methods that are suitable for predicting the response of Li-ion batteries to high-energy impact, crash, and blast events at a reasonable computational cost. In particular, an efficient method is developed for ballistic M&S of Li-ion batteries by using a Thick Shell Composite (TSC) representation of Li-ion batteries using the commercially available FEA software, LS-DYNA. This approach shows promise for modeling the battery at the module or full-pack level with significantly reduced computational cost compared to a more traditional modeling approach. Individual layers are embedded into this TSC in order to reduce the number of finite elements in each cell significantly.

In order to test and validate the M&S approach, a model of a generic but representative battery pack is built and integrated with a steel casing model. This is a notional system that does not represent a specific battery mounted in a particular ground vehicle. However, from a numerical perspective, it does entail the same high level of computational demands that would be required to simulate an actual vehicle-mounted battery system. This generic battery model has therefore been used for research purposes to run initial ballistic simulations for an integrated battery-vehicle structure, in order to examine the computational efficiency of various approaches, as well as to establish standard procedures and best practices for future M&S efforts. In particular, the M&S analysis method presented in this paper focuses on the system-level mechanical failure of batteries due to high-speed bullet impact, which is very challenging to capture from a computational perspective.

PROBLEM STATEMENT

A battery is made up of many cells that are combined in series and/or parallel into modules. These modules are then combined in a full battery pack. There are different form factors for battery cells. In this paper, pouch cells are considered, which have a plate-like form factor.

A single pouch cell is typically comprised of 16 to 24 layers, with the precise number depending upon capacity and

size requirements. The notional battery system used in this study has 24 layers in each pouch cell.

Figure 1 shows the sub-layer thicknesses of a single layer in the Li-ion battery cell. The average thickness of the full layer is 265 microns (0.265 mm). One cell with 24 layers plus the pouch material is approximately 7.2 mm thick.

Positive Current Collector (Aluminum foil) = 20 μ	ONE LAYER
Graphite Anode = 95 μ	
Separator (Polypro) = 20 μ	
Electrolyte NaCl = 20 μ	
LiFePO4 Cathode = 100 μ	
Negative Current Collector (Copper foil) = 20 μ	
Separator (Polypro) = 20 μ	

Figure 1: Single layer of a Li-ion battery cell.

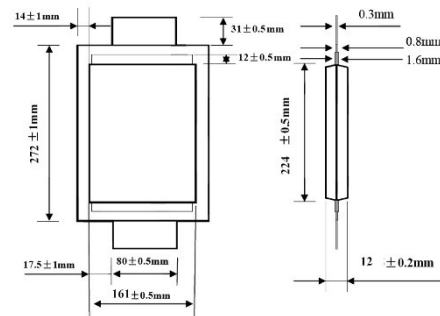


Figure 2: Dimensions of a pouch cell (24 layers).



Figure 3: One module consisting of 12 pouch cells in series.

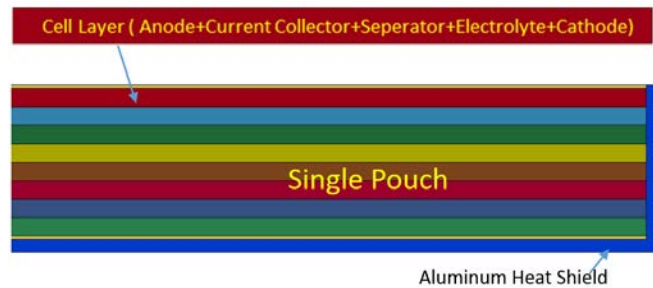
Figure 2 shows the dimensions of a single pouch cell. Figure 3 shows one module of the generic battery model with 12 cells in series. This configuration requires over one million finite elements to represent one layer of the pouch cell and over 24 million elements for one pouch cell. Computationally, it is very challenging to run such a large

model even at the single-cell level. With this approach, the full pack would have over 100 million elements, which makes it extremely challenging or even impossible to carry out simulations with the available resources.

Therefore, meshing the cells at the micromechanical scale may not be the best approach. However modifying the original CAEBAT [2, 3] model may work for a single cell, or for a few cells, but it becomes infeasible for a module or a full pack. This is especially true for models to be used for system-level bullet penetration simulations, given the very large number of elements associated with these models. As an alternative approach, one could represent the complex Li-ion cell materials as an equivalent homogeneous material and model as a single thickness layer. However, this requires an equivalent or homogeneous material property for the single-cell configuration, which may or may not provide the true or best behavior of the materials at high-strain, high-speed impact loading.

In this paper, a new approach is proposed, which is called the System Level Ballistics Simulation Method for Li-ion Batteries. The key idea is to represent a single cell layer as a thick shell composite (TSC) in LS-DYNA [4] with one integration point for each material. By adopting this strategy, all of the different materials are represented independently at the microscale at each layer. This approach seeks a balance between fidelity and cost: it eliminates the limitations due to simplifying assumptions associated with a homogeneous representation of complex materials in Li-ion batteries, yet it also provides a way to represent a module with much fewer than the approximately 20 million elements required for a more detailed finite element representation.

NUMERICAL MODELS



```
*PART_COMPOSITE_TSHELL
$# PID elform shrf unused unused hgid unused tshear
$# mid1 thick1 b1 tmid1 mid2 thick2 b2 tmid2
1 2 0.000 0 1 0
1 2.0000E-5 0.000 0 2 9.5000E-5 0.000 0
3 2.0000E-5 0.000 0 4 1.2500E-4 0.000 0
1 2.0000E-5 0.000 0 2 9.5000E-5 0.000 0
3 2.0000E-5 0.000 0 4 1.2500E-4 0.000 0
```

Figure 4: Single pouch cell model (top) and corresponding thick composite shell card in LS-DYNA (bottom).

Pouch Cell Model

Figure 4 shows the single pouch cell modeled as a TSC. Each pouch cell model has 2.5 million elements. A thin shell element model of the single pouch cell resulted in 12.5 million elements.

The LS-DYNA *PART_COMPOSITE_TSHELL card, which is shown at the bottom of Figure 4, captures the thickness of each integration point and provides the capability to input thermal material properties and material angles as well. The first line represents the part definition and element formulation. The second line represents the layer definition as integration points such as thickness, material angle, thermal material identification numbers, and mechanical material identification numbers.

The geometry of the pouch cell analyzed in this project is 272 mm in length and 161 mm in width. The thickness of the pouch cell is 7.21 mm, including the outside pouch material.

Module Model

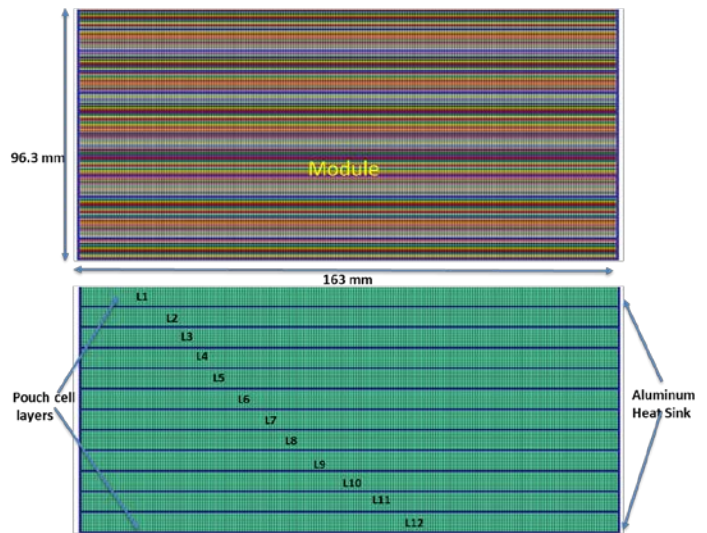


Figure 5: Single module model.

Figure 5 shows the single module model using TSC. Each pouch is separated by an aluminum heat shield and stacked as a layered sandwich. This model has 30 million thick shells comprising of 12 pouch cells. This is sufficient to capture local damage for a ballistic simulation. The equivalent thin shell model would have resulted in 150 million elements, which is a five-fold increase in model size.

One pouch cell has 144 layers and one module has 1,768 layers. In addition to these 1,768 active component layers, the module has a heat sink between pouch cells. These heat sinks are made of 0.5mm aluminum. There are 13 layers of these aluminum heat sinks. The heat sink is modeled in this project as 8-node hex solid elements with single point integration constant stress element formulation. Since the problem involves very high speed and high strain, analysis may result in spurious energy modes. To mitigate this *HOURLASS is activated with default values which is viscous formulation.

Bullet Model

Figure 6 shows the NATO 0.308 full metal jacket caliber with 7.62 mm in diameter and 51 mm in length.

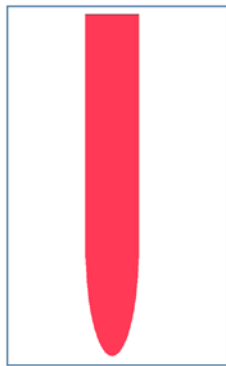


Figure 6: NATO 0.308 Caliber bullet model.

During impact, the tip of the bullet and the bottom of the bullet may exhibit extreme deformation and could result in material erosion. Since the bullet is modeled using a Lagrange element formulation, material points and nodal points coincide and they move together. In some extreme deformation cases, this may create numerical instabilities. In order to avoid this numerical instabilities, additivity has been used for the bullet model: when any part of the bullet material fails, it will be converted into smooth particles and inherit the properties of the parent material.

The *DEFINE_ADAPTIVE_SOLID_TO_SPH option in LS-DYNA allows failed solid elements to be converted into smooth particles. It is computational expensive and requires significant memory as well. Nevertheless, it is worth the cost due to the complexity of the problem being analyzed. The user has the option of converting a failed element into 1, 9, or 27 smooth particles. In this analysis, this is set to 1 smooth particle because each Lagrange element is 0.5 mm.

Material Properties

Table 1. Material properties summary

Mechanical Property	Units	Aluminum Current Collector	Copper Current Collector	LiFePO ₄	Separator	Graphite Anode	Brass Bullet
Density	kg/m ³	2,700	7,983	2,600	1,176	2,200	10,822
Elastic Modulus	MPa	70,000	110,000	12,500	3,450	32,000	115,000
Yield Stress	MPa	195	230	10	180	97	896

Since this work is a continuation and extension of research conducted by the DOE National Renewable Energy Laboratory (NREL) under a previous CAEBAT project, most of the materials properties used in this analysis were taken from the results of that project. In particular, the properties used in this study for a LiFePO₄ cathode material were reported in [5-7] and are summarized in Table 1.

VALIDATION FOR POUCH CELL TESTS

In the CAEBAT project carried out by NREL, physical tests were conducted for two pouch cells in series. Figure 7 shows the physical test setup. Two pouch cells were held together by a clip supported from two vertical fixed poles diagonally. The other two diagonals were clipped to keep the pouch cells intact before the test.



Figure 7: Physical test setup.

In order to validate the new TSC methodology, a numerical test for the two-cell system was run and compared to the physical tests. Figure 8 shows the numerical test setup. Numerically, the clips were represented as constrained boundaries by applying single point constraints (SPCs) to several boundary degrees of freedom in LS-DYNA. The locations of these SPCs are indicated in Figure 8.

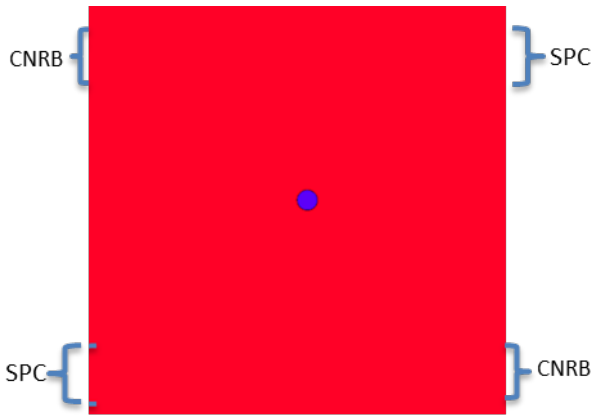


Figure 8: Numerical test setup.

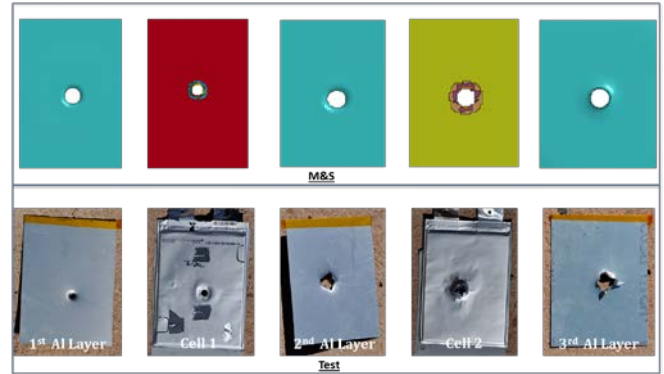


Figure 10: Bullet impact test – cell layer deformations.

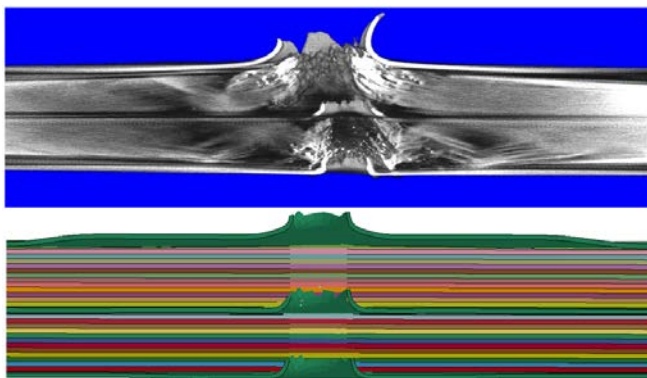


Figure 9: Physical test (top) versus simulation (bottom).

Figure 9 shows the results from the numerical simulations compared to those from the physical test. Numerical simulation captures the bullet kinematics and perforation of the battery cells very well.

The deformation of various internal layers are shown in Figure 10. It is seen that there is very good agreement between the TSC simulation results and the physical test results with respect to capturing both the extent of the local damage and the patterns of the deformation.

SIMULATION RESULTS FOR MODULE TESTS

Having validated the numerical approach with the two-layer pouch cell tests, the next step was setting up impact model for a full battery module. Three different loading conditions were analyzed: 45 degree oblique loading, 90 degree vertical loading, and horizontal loading. Figure 11 shows the three loading conditions. The battery module is enclosed in a plastic casing and bolted on to steel casing made of RHA material. The steel casing in this analysis represents a generic vehicle structure that may be exposed to external threats such as a bullet strike.

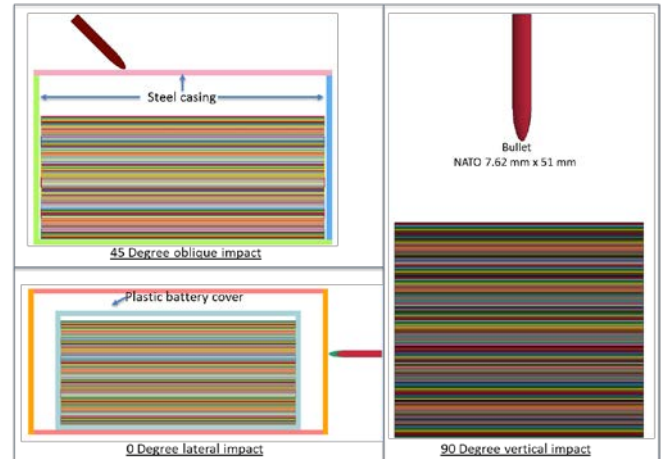


Figure 11: Three loading conditions for a single module.

The objective of this analysis is to understand how far the bullet will penetrate into the battery module when exposed to such loading. Only mechanical failure of the battery cells and structure is analyzed in the study. Initial velocity of the bullet in all the three loading conditions is set at 825 m/s.

Battery cell deformations and structure deformation are shown in Figure 12 for the oblique impact loading. Bullet

penetrated 50% of the battery module in oblique loading case with an angle of 45 degrees.

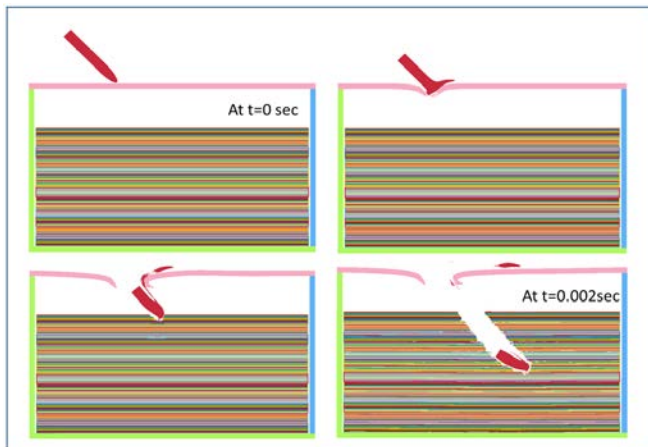


Figure 12: Simulation results for oblique impact.

For the vertical impact loading case, the bullet penetrates 80% of the battery module, as shown in Figure 13. Figure 14 captures the cell deformations of horizontal impact loading. During horizontal loading, the bullet penetrates 45% of the cell layers. Also note that in horizontal loading only two or three pouch cells are affected, as opposed to many layers in vertical and oblique loading.

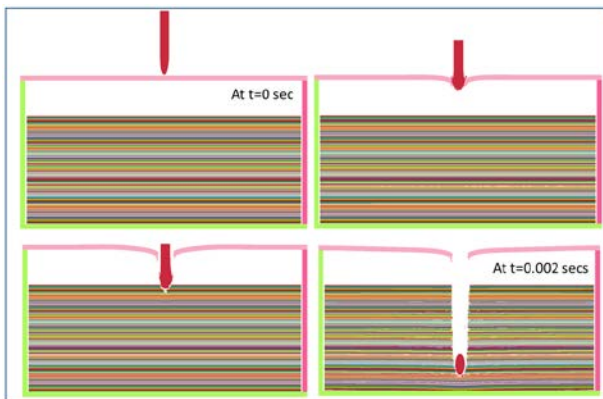


Figure 13: Simulation results for vertical impact.

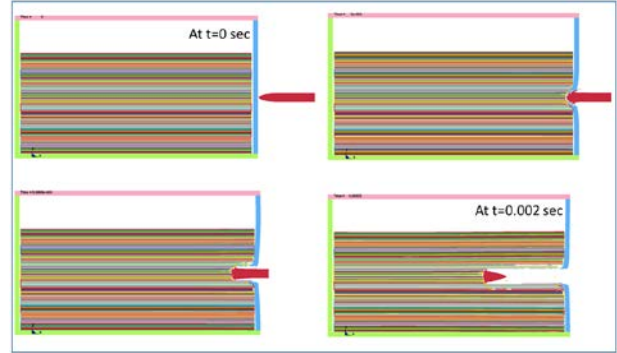


Figure 14: Simulation results for horizontal impact.

Bullet velocities are shown in Figure 15 for all the three loading conditions. Cell layers exhibit lower stiffness in horizontal directions, resulting in faster bullet penetration and eventually stops at 170 m/s. Higher cell layer stiffness results in slower penetration of the bullet both in oblique and vertical loading. Vertical bullet velocity stops at 220 m/s and oblique bullet impact stops at 190 m/sec.

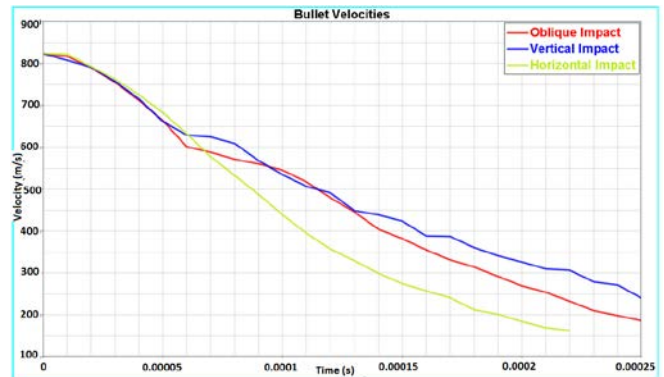


Figure 15: Bullet velocities for the three impact cases.

In all the three cases of loading, the bullet penetrates at least 40% of the module. Figures 12-14 show that the TSC model captures the strong deformation of the pouch cells under these loading conditions.

In addition to the deformation, the shock waves from the bullet impact cause damage to the electrodes. This damage could then potentially lead to high temperatures and thermal runaway, which are not captured in this analysis. These effects will be considered in future work.

CONCLUSIONS

A new approach for modeling a module or a full pack of a Li-ion battery has been presented in this work. The new method uses Thick Shell Composites (TSC) in the

commercial software package LS-DYNA. First a two pouch cell numerical model was developed using thin shells with 12.5 million elements, and the simulation results were correlated with those from bullet impact physical tests. An equivalent TSC method was developed with 2.5 million elements and correlated to the same tests and extended to a battery module consisting of 12 pouch cells. These 12 cells have a total of 1768 layers consisting of positive and negative current collectors, anodes, cathodes, separators, and electrolytes stacked in series. The battery module was enclosed in a plastic casing and bolted to a generic vehicle structure with RHA used as the structural material. This single module LiFePO₄ battery was subject to three ballistic loading cases: 45 degree oblique impact, vertical impact, and horizontal impact loading with NATO 0.308 short caliber at 825 m/s initial velocities. The mechanical damage incurred by the battery layers due to the bullet impact were assessed for all the three loading conditions. The TSC model captured the strong anisotropic deformation of the battery cells.

The main objective of this work was to develop a finite element modeling method to simulate the ballistic response (bullet impact, crash, etc.) of a Li-ion battery and assess the attendant mechanical failures. The microscale thicknesses of the layers in each battery cell make it numerically very challenging to represent each layer at that scale and still be able to analyze the full battery module or pack at the macroscale level without incurring prohibitive computational costs. Proceeding with a traditional finite element modeling approach would have required well over 100 million elements and 600 million degrees of freedom for the numerical example considered, which would pose a daunting numerical challenge. In contrast, the proposed TSC approach allows us to model multiple layers of batteries with relatively few elements compared to the traditional model while retaining very good accuracy. Further development is in progress to couple the electrical, chemical, and thermal response with the mechanical response in the TSC model.

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