Numerical Model for Characterization of Multifunctional Energy Storage Composite Cells, Modules, and Systems

YINAN WANG, PURIM LADPLI, FOTIS KOPSAFTOPOULOS
and FU-KUO CHANG

ABSTRACT

Recent work on multifunctional materials has demonstrated that high-strength composites could be integrated with active Li-ion battery material to create high strength and high energy density storage structures that could meet the transportation requirements on mobility and energy storage density. However, the performance and the design of the multifunctional materials require fundamental understanding of the mechanical behavior of the integrated Multifunctional Energy Storage (MES) Composites systems under various loading conditions. Characterization of this new class of multifunctional materials would become very challenging without an adequate simulation model to guide the tests and validate the results.

Therefore, this work presents the mechanical simulation and design of the MES Composites system that consists of multiple thin battery layers, polymer reinforcements, and carbon fiber composites, which results significant challenges in simulation and modeling. To tackle these issues, homogenization techniques were adopted to characterize the multi-layer properties of battery material with physics-based constitutive equations combined with non-linear deformation theories to handle the interface between the battery layers. Second, both mechanical and electrical damage and failure modes among battery materials, polymer reinforcements and carbon fiber-polymer interfaces were characterized through appropriate models and experiments.

The model of MES Composite has been implemented in a commercial finite element code. A comparison of structural response and failure modes from numerical simulations and experimental tests will be presented in the paper. The simulated strain distribution and its application to Structural Health Monitoring (SHM) on MES Composites will also be discussed. The results of the study showed that the predictions of elastic and damage responses of MES Composites at various loading condition agreed with the test data. With appropriate material parameters determined from experiments, this multi-physics model can be used as a necessary tool to characterize a failure envelop that governs the design of MES Composites under specified electrical and mechanical loads.

Yinan Wang, Purim Ladpli, Fotis Kopsaftopoulos, Fu-Kuo Chang, Stanford University, Department of Aeronautics and Astronautics, Stanford, California, USA, 94305

INTRODUCTION

Electrical Vehicles (EV) has been widely accepted in automotive industry as the solution to improve fuel economy and reduce emissions. Lithium-ion batteries are used in most applications due to their high energy density, but are not as robust as some other rechargeable technologies. Even the state-of-the-art Lithium-ion batteries add significant weight to vehicles both in the form of battery weight and supporting systems. This weight significantly hinders vehicle performance and efficiency. A primary source of the penalty is that the battery packs and supporting structures each serve only one purpose, i.e. energy storage or load bearing. These issues motivated researchers to develop multifunctional battery materials and configurations for additional weight saving. Among many research ideas, Structures and Composites Laboratory (SACL) at Stanford University has developed Multifunctional Energy Storage (MES) Composites cells and systems that combine Li-ion battery materials and carbon fiber composites in a novel approach [1]. Through unique design and fabrication processes, MES Composites are proven to be able to store electrical energy as well as taking mechanical loads. Unlike traditional EV battery packs, the battery material within MES Composites undertakes significant mechanical stress during operation [1]. The need to fully understand the material properties and behavior under various loading conditions motivated the proposed research of numerical simulation on MES Composites.

In the past, various attempts have been made to model the mechanical behavior of battery cells and battery packs. Sahraei et al. modeled jellyroll and pouch cells as compressible foam with a homogenized isotropic constitutive behavior and validated with punch and bending tests [2, 3]. Ali et al. adopted Gurson's material model to account for the effect of porosity in separator and electrode sheets under constrained compression [4]. Greve and Fehrenbach successfully predicted fracture and the initiation of an internal short circuit by using a macro-mechanical model based on the classical Mohr and Coulomb criterion [5]. However, these models and approaches are only capable of modeling the global mechanical response of batteries in simple configurations, either pouch or jellyroll, and failed to address the interactions between battery layers and surrounding materials.

This paper presents the development of a simulation model that can accurately predict the mechanical behavior of MES Composites from coupon level, cell level, module level, all the way to system level. The model has detailed cell configuration and interface interactions below module level and is able to provide stress/strain/damage distribution within every component of the multifunctional material. Homogenization techniques are used to model MES Composites beyond system level to reduce computational cost. Given appropriated material properties and desired loading and boundary conditions, this parametrized model can provide system-level stiffness, deflection, as well as strain distribution in composite facesheets. The model of MES Composites has been implemented in a commercial finite element code. A comparison of structural response and failure modes from numerical simulations and experimental tests has been studied. The results of the study showed that the predictions of elastic and damage responses of MES Composites at various loading condition, such as bending, tensile, and compression tests, agreed with the test data.

METHOD OF APPROACH

In order to understand the mechanical behavior of MES Composites, initial set of experiments were conducted on all components, including battery layers in a pouch cell form, carbon fiber facesheets, and Polyethylene coupons. Based on the experimental findings, an elastic-plastic model was used to simulate MES Composites cells and modules under different loading conditions. Next, a series of experiments were conducted to validate the numerical model. Last, a design and parameterized model was developed to optimize mechanical behavior in any given loading and power requirement.

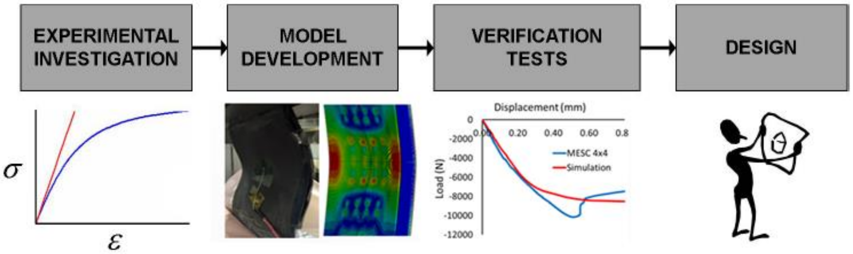


Figure 1. Method of approach.

MATERIAL MODEL

Composite Facesheet

MES Composites can take different types of materials as facesheet, such as laminate/woven carbon fiber composites, aluminum, glass fibers, etc. In this paper, carbon fiber facesheets are used and modeled as laminate composites with Hashin failure criteria. Laminate composite material models are presented despite that woven composite is more frequently used. Woven material models are also being used for large deformation and crush simulations [6]. This paper address mostly the linear response of the MES Composites cells and modules. A general orthotropic constitutive equation is listed below, which is sufficient to model the linear behavior. The stiffness matrix is obtained by taking the inverse, and transferred into local coordinates. The Hashin failure criteria is used as an indicator of the initial failure of composite. The parameters are obtained from tensile tests of facesheet coupons for both $[0/90]_3$ and $[\pm 45]_3$ layers. The experimental and simulation results are shown below. The Young's Modulus are directly obtained from the slop of the curve and the shear modulus are calculated according to ASTM D3518/D3518M.

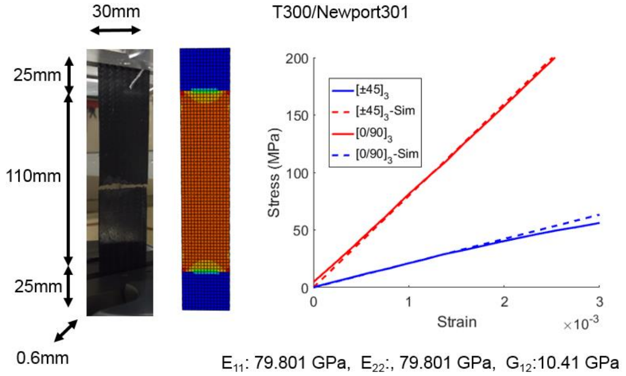


Figure 2. Facesheet coupon tensile test and simulation results.

Polyethylene Frame and Rivets

PE material is currently modeled as linear isotropic material. Even though it has plastic response in large deformation, it is ignore because the overall mechanical contribution from PE is low. The plasticity only affects MES Composites in large deformation or crush, which is not presented in this paper. The tensile tests below gives an estimate Young's Modulus of 350 MPa, which agrees with results from other researchers [7].

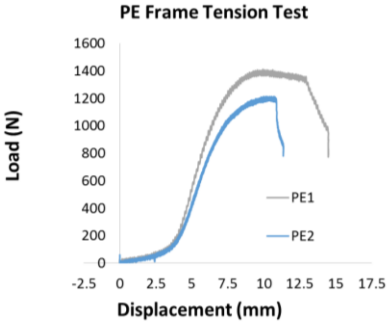
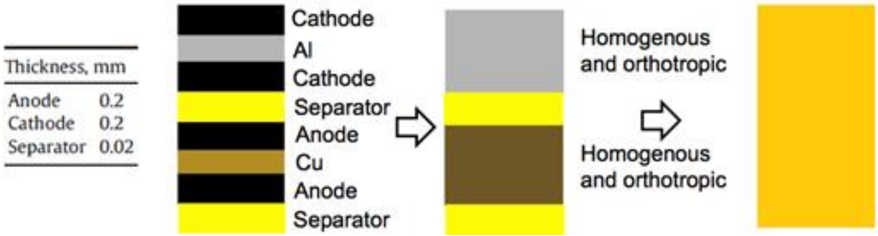


Figure 3. Polyethylene coupon tensile test results.

Battery Homogenization

Active battery material consists of repeated thin layers of electrodes and separators. Homogenization is commonly used to model the mechanical behavior of the overall battery stack. Current most state-of-the-art modeling techniques assume the material to be homogeneous and isotropic, with data fitting techniques such as power law. This approach is relatively easier to model and provides a fairly accurate result for global behavior. However, they require unique material properties for different configurations, such as small or large pouch cells, despite of having the same material. The model in this paper also first takes a homogenization approach [8], but the constitutive relation varies to take account the softening between battery layers under large deformation.



Thickness, mm	
Anode	0.2
Cathode	0.2
Separator	0.02

Figure 4. Battery homogenization scheme [8].

After homogenization, the active battery material is modeled as non-linear orthotropic material as shown below. It has different properties in each direction, as well as varying out-of-plane shear modulus that are suitable for any configuration. For linear mechanical response, battery material has a similar formulation as composite, since they are both orthotropic. The battery material has a much lower out-of-plane shear modulus due to lack of lamination or bonding between layers. Most of the structural integrity is provided by the surrounding structures, such as facesheet, rivets and frames. For small deformation of MES Composites under mechanical loads, the contribution from the nonlinear term $\alpha_{ij}\sigma_{ij}^3$ becomes insignificant. The model can be drastically simplified by setting α_{ij} to zero, resulting a traditional orthotropic model as composite. For large deformations, such as crushing, the model will have non-linear behavior, which will result in a varying shear modulus based on given applied out-of-plane stress distribution, additional α_{ij} are needed to model in such phenomenon. The results of the parametric study will be presented in the future. The compliance is then inverted and transferred into local coordinates. Similar to facesheet, the modulus of homogenized battery stacks in this model is calculated from tensile test results of smaller MES Composites coupons, discounting the contribution from facesheets.

$$\begin{Bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{23} \\ e_{13} \\ e_{12} \end{Bmatrix} = \begin{bmatrix} 1/E_1 & -\nu_{12}/E_1 & -\nu_{13}/E_1 & 0 & 0 & 0 \\ -\nu_{12}/E_1 & 1/E_2 & -\nu_{23}/E_2 & 0 & 0 & 0 \\ -\nu_{13}/E_1 & -\nu_{23}/E_2 & 1/E_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{12} \end{bmatrix} \begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{Bmatrix} + \begin{Bmatrix} 0 \\ 0 \\ 0 \\ \alpha_{23}\sigma_{23}^3 \\ \alpha_{13}\sigma_{13}^3 \\ 0 \end{Bmatrix} \tag{1}$$

$$e_{23} = \frac{1}{G_{23}}\sigma_{23} + \alpha_{23}\sigma_{23}^3 \qquad e_{13} = \frac{1}{G_{13}}\sigma_{13} + \alpha_{13}\sigma_{13}^3 \tag{2}$$

Component Interface

There are four types of interactions between different parts: they are facesheet-polymer, battery-frame, battery-rivet, and battery-facesheet. Battery and carbon fiber interface are non-sticky, so tangential and normal contact properties are used in the model. Tangential contact is modeled as classical isotropic Coulomb friction. It assumes that no relative motion occurs for the linear part of the deformation. Normal contact is modeled as the penalty Lagrange constraint enforcement. Polymer and facesheet are melted together during manufacturing. The bonding can be modeled as cohesive properties between two parts. The elastic traction-separation law with damage initiation and evolution laws are used to govern the behavior of the cohesive behavior.

FEM IMPLEMENTATION AND MECHANICAL TEST RESULTS

The flowchart below summarizes the overall approach of the modeling techniques. This follows a typical material development in Finite Element Code, such as ABAQUS, with the unique methods in the middle boxes. The battery model generates the homogenization scheme and the constitutive law to govern the mechanical behavior of the battery layers as mentioned above. The interface model, on the other hand, controls the linear and failure states between battery-CF, battery-PE, and CF-PE interfaces. The parameters are calibrated in the coupon and cell-level tests, and are directly applied to the module and system-level simulations. The model is able to simulate MES Composites in any architecture and configuration. Results of 4x4 rivet distribution are chosen in this paper.

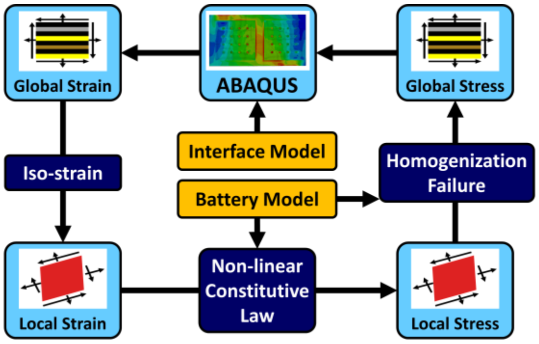


Figure 5. FEM implementation overview.

Cell-level Testing and Simulation

First, an MES Composites cell is cut open to investigate the mechanical behavior under three-point-bending load. Figures below show the number of samples prepared with their dimensions and the test setup. The samples are subject to three-point-bending in the MTS machine, with loading speed about 0.01mm/s, sufficiently slow for quasi-static approximation.

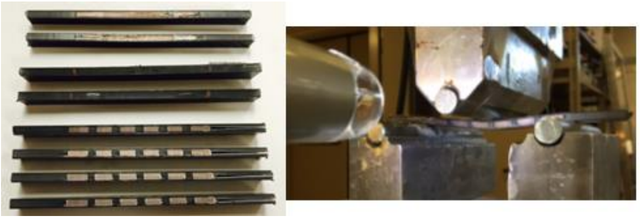


Figure 6. Cut MES Composites strips and test setup.

Figures below show the load and displacement curves for each couple under the aforementioned loading condition. It is apparent that the experiments are repeatable, especially in the linear region (beginning part of the curves). The strips with PE cores have the strongest bending stiffness, as well as the highest strengths. The riveted strips show significant improvements over the non-riveted cases. The linear region is taken below and compared with simulation results that were done previously. It shows an agreement of greater than 80%.

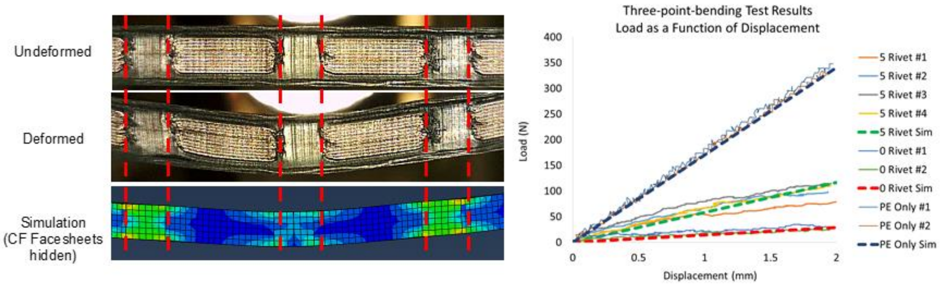


Figure 7. Cut MES Composites strips bending test results.

Next, MES Composites cells are tested under bending, tensile and compression. The experiments were conducted on multiple cells, both electrically live and dead. The results show great repeatability. Strain gauges are mounted in the middle of the sample to obtain strain measurements, which are then used to calculate the sample displacement. Within expected range of loads that are likely to subject on the cells, linear behavior is observed. The simulation results show great agreements of more than 90%. Under such loads, no mechanical or electrical failure is observed. Upon further loading, multiple failure modes starts to occur mechanically.

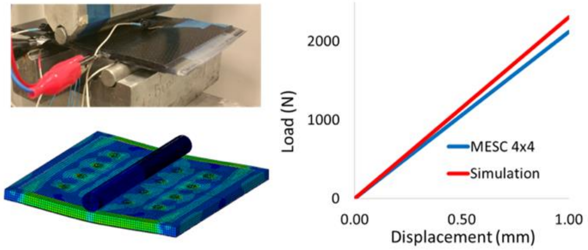


Figure 8. MES Composites cell bending test results.

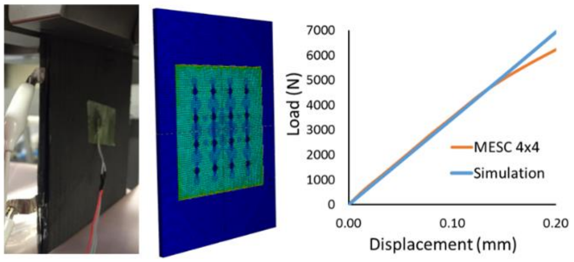


Figure 9. MES Composites cell tensile test results.

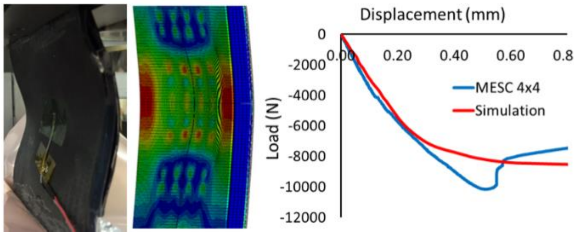


Figure 10. MES Composites cell compression test results.

Module-level Testing and Simulation

Two multi-cell MES Composites module are fabricated and subject to a three-point bending load. Due to the complexity of the module, large number of elements are needed to fully capture the detail of each component. A quarter beam model with symmetrical boundary conditions is created for simplicity. There are about 300000 elements with a mixed type of C3D8R, SC8R, and C3D6 in Abaqus. Strain gauges are mounted on the beam and the location are shown in red circles and the strain measurements are used to validate the model.

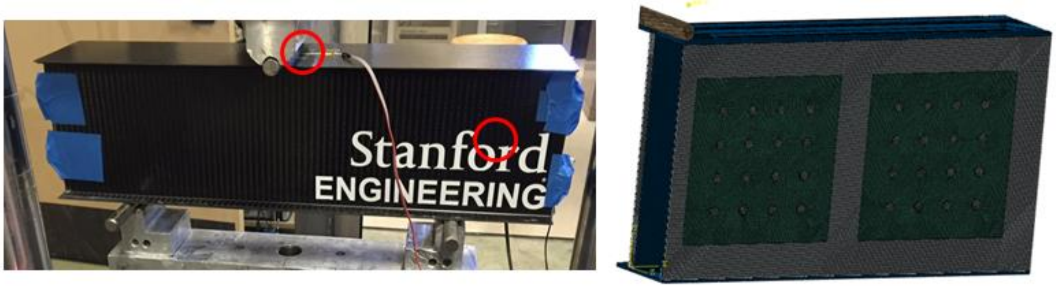
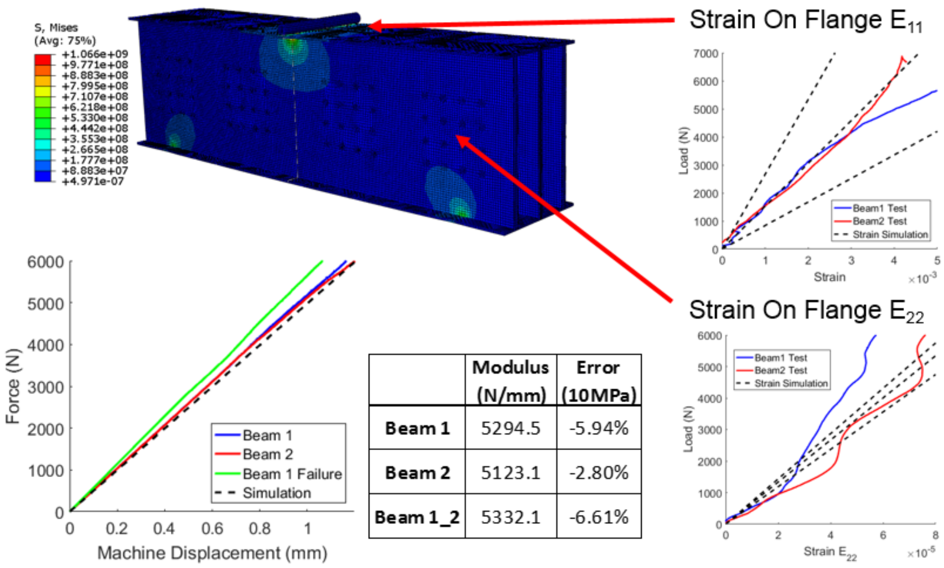


Figure 11. MES Composites module three-point-bending test setup.

Initial tests showed that the module is softer than we expected. The main reason is that the top flange of the module are glued with the webs, instead of co-cured. An additional layer of soft bonding material is introduced in the numerical model to take account the softening. The modulus of this thin layer is set to close to zero. After this adjustments, the load and displacement curve of the simulation agrees with the experiment within 7% as shown below. For the strain measurements and simulation, we have observed that the strain distribution has a large variance across small change of location, even between two adjacent elements. This is because the beam has a relative short span compared to its height. The back lines in the figures below show a bound of possible simulated strain, with the middle line being the element that’s the most close to the real location. The non-linearity of the strain measurements are the results of manual fabrication errors of bonding all components together.

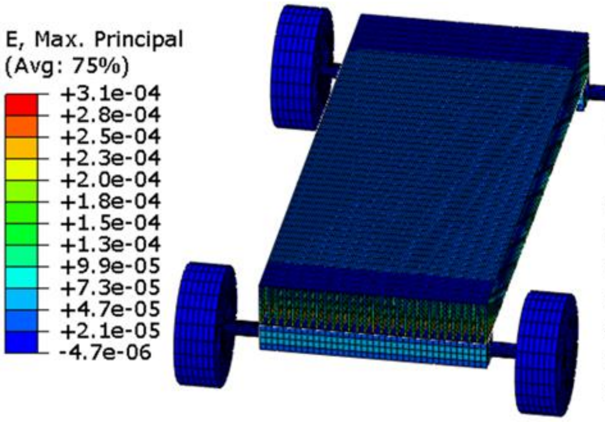


	Modulus (N/mm)	Error (10MPa)
Beam 1	5294.5	-5.94%
Beam 2	5123.1	-2.80%
Beam 1_2	5332.1	-6.61%

Figure 12. MES Composites module three-point-bending test results and simulation.

System-level Simulation and Design

The system-level simulation is also an on-going effort of development. The current design of the system is the floor of an EV of similar size as a Tesla Model S. The design is also based on a similar battery capacity of 85 kWh. The current full-scale model is simplified and no rivets are present due to computational limit. This will provide a guideline for normal operation condition and a rough estimate on the total weight saving. As the diagram shown below, the MES Composites battery pack sits on two axels of the vehicle and carries the body weight of the car and the passengers of total 1.5 ton. This is the static condition as a parking car would experience. From the first order of estimate, a maximum 0.03% principle strain is observed around the pack-axel joint, and a much lower strain inside the battery cells. It is within a safe range of the material limit. This gives a total weight of 500 kg, which is about 30% weight saving compared with a Tesla battery pack of 85 kWh. The specification of such a system is also given below. It is important to notice that this design is not the optimized design, but rather a starting point of a full-scale design. The final design would have a similar, but different dimension. Other loading conditions, such as a dynamic load and frontal load are also being studied.



Dimension: 1.3m x 2.7m x 0.2m
Capacity: 85 kWh
Weight: 500 kg
Load: 1.5 ton even distribution
Support: two-axle support
Max. Deflection: 0.67 mm
Max. Principle Strain: 0.03%

Figure 13. Full-scale simulation for a MES Composites battery pack of 85kWh.

Application of SHM on MES Composites

The previous development from Ladpli et al. has shown that MES Composites utilize in-situ integration of sensor/actuator networks to enable battery and structural health monitoring capabilities [9]. In addition to the strain gauges mentioned above, SHM-based ultrasonic inspection techniques have been adopted for battery health prediction of MES Composites under static state (Figure 14). In reality, MES Composites will become a part of the structure that constantly takes mechanical load during operation. Research has shown that structural loads have significant influence on piezo-sensor signals [10]. The simulation model, together with the strain gauges, helps to predict the strain distribution of the entire cell, module, and/or system. As a result, proper load compensation techniques can be used for more accurate state-awareness of batteries. In addition, this simulation tool provides a framework for numerical training of the MES Composites for passive impact reconstruction. Similar research has been done previously by SACL members on impact identification of composite panels [11], and the theories can be directly transferred to the MES Composites.

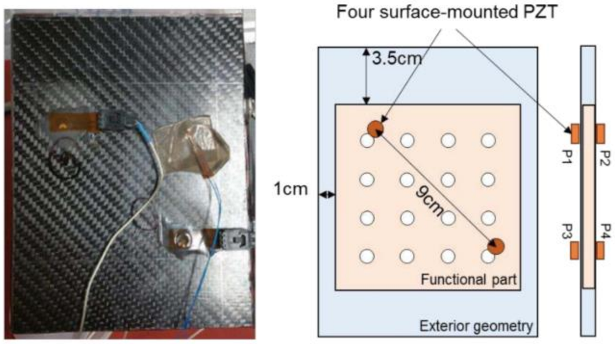


Figure 14. Piezoelectric transducers mounted on the MES Composite cell [9].

CONCLUSION

A mechanical simulation model of MES Composites has been presented in this paper. Each component of MES Composites are modeled with appropriate methods and the interactions between each component are defined. The model covers from cell level, module level, all the way to system level. Experiments were conducted on MES Composites cells and modules as validation. The results showed promising agreements. The main results and future research are shown below:

- The mechanical configuration of MES Composites cells has significantly increased the stiffness of the battery, observed from both experimental and simulation results. The stiffness changes for different architectures, such as rivet size, and the simulation tool is able to capture this effect.
- Under a significant amount of mechanical load, MES Composites cells and modules still behave linearly elastic, which further substantiates the mechanical rigidity of the design. Upon further loading, the cells will eventually break mechanically, followed by electrical failures.
- From system-level analysis, an EV-sized MES Composites battery pack can save around 30% weight compared to the state-of-the-art automobiles in the market.
- Post failure and crush analysis will be the next step to complete the development of this numerical tool.

REFERENCES

1. Ladpli, P., Nardari, R., Rewari, R., Liu, H., Slater, M., Kepler, K., Wang, Y., Kopsaftopoulos, F. and Chang, F.K., 2016, June. MULTIFUNCTIONAL ENERGY STORAGE COMPOSITES-DESIGN, FABRICATION, AND EXPERIMENTAL CHARACTERIZATION. In *ASME 2016 Power & Energy Conference, Charlotte, NC, USA.*
2. Sahraei, E., Meier, J. and Wierzbicki, T., 2014. Characterizing and modeling mechanical properties and onset of short circuit for three types of lithium-ion pouch cells. *Journal of Power Sources*, *247*, pp.503-516.
3. Wierzbicki, T. and Sahraei, E., 2013. Homogenized mechanical properties for the jellyroll of cylindrical Lithium-ion cells. *Journal of power sources*, *241*, pp.467-476.
4. Ali, M.Y., Lai, W.J. and Pan, J., 2013. Computational models for simulations of lithium-ion battery cells under constrained compression tests. *Journal of Power Sources*, *242*, pp.325-340.
5. Greve, L. and Fehrenbach, C., 2012. 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*, *214*, pp.377-385.
6. Flesher, N.D., Chang, F.K., Janapala, N.R. and Starbuck, J.M., 2011. A dynamic crash model for energy absorption in braided composite materials-Part II: Implementation and verification. *Journal of Composite Materials*, *45*(8), pp.867-882.
7. Rocha, M.C.G., Leyva, M.E. and Oliveira, M.G.D., 2014. Thermoplastic elastomers blends based on linear low density polyethylene, ethylene-1-octene copolymers and ground rubber tire. *Polímeros*, *24*(1), pp.23-29.
8. Qin, Q.H. and Yang, Q.S., 2008. *Macro-micro theory on multi-field coupling behavior of heterogeneous materials*. Springer,
9. Ladpli, P., Nardari, R., Kopsaftopoulos, F., Wang, Y. and Chang, F.K., 2016. Design of Multifunctional Structural Batteries with Health Monitoring Capabilities. In *European Workshop on Structural Health Monitoring*.
10. Roy S, Ladpli P, Chang FK. Load monitoring and compensation strategies for guided-waves based structural health monitoring using piezoelectric transducers. Journal of Sound and Vibration. 2015 Sep 1;351:206-20.
11. Mueller, I., Larrosa, C., Roy, S., Mittal, A., Lonkar, K. and Chang, F.K., 2009, September. An integrated health management and prognostic technology for composite airframe structures. In Proc. Annual Conference on Prognostics and Health Management.