CONCEPTUAL DESIGN FRAMEWORK FOR LAMINATED STRUCTURAL BATTERY COMPOSITES

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Abstract
The structural battery composite is a class of composite materials with ability to provide mechanical integrity in a structural system while simultaneously store electrical energy (i.e. work as a battery). In this paper a framework to estimate the mechanical and electrical performance of laminated structural battery composites is proposed. The mechanical performance of the battery composite laminate is assessed by estimating the in-plane elastic properties of the laminate using Classical Laminate Theory. The electrical performance is assessed estimating the specific capacity and energy density of the component. The developed framework is applied on an A4 sized structural battery composite demonstrator, as part of the Clean Sky 2 project SORCERER [1] to demonstrate the capabilities of the framework. The design process for the demonstrator is presented and mechanical and electrical performance metrics are estimated for three laminate configurations, one promoting structural performance, one promoting electrical performance and one intermediate. As the material provides both load carrying and electrical energy storage capabilities, the laminate configuration can be alternated to provide suitable performance based on the purpose of the component.

1. Introduction

A route to high-performance lightweight electric vehicles is smart vehicle designs, utilizing multifunctional materials such as structural battery composites. The structural battery composite is a composite material with ability to provide mechanical integrity in a structural system while storing electrical energy. This composite material is a multifunctional material, which means that it can perform multiple functions, hence fulfilling mechanical demands as well as storing energy. Due to its multifunctionality, the structural battery composite material is often referred to as “massless” energy storage [1], subsequently providing significant weight reduction on a system level [2]. The structural battery is particularly important for the electrification of transportation vehicles such as electric aircraft and cars as it has the potential to revolutionize future design of lightweight electric vehicles. Airbus, who is a leading aircraft producer, aspires to make all-electric regional aircraft by 2050. In order to do this, new energy storage solutions are needed. Due to the low energy to weight ratio of existing monofunctional battery technologies, unrealistically high energy storage per passenger is needed. Structural battery composites provide a potential solution to this problem, adding “mass less” energy storage within the structural system. In addition to energy storage, the material provides a possibility to distribute the energy stored, reducing the need for cables, further lowering the weight of the aircraft. Consequently, this material can have significant impact on sustainable transportation meeting future requirements on reduced emissions.

In this paper a novel framework to estimate the multifunctional performance of laminated structural battery composites is presented. The mechanical performance is assessed by estimating the in-plane elastic properties of the laminate using Classical Laminate Theory and the electrical performance is assessed estimating the specific capacity and energy density of the component. The developed framework is applied on three cell designs for an A4 sized structural battery composite demonstrator, as part of the Clean Sky 2 project SORCERER [1], to demonstrate the capabilities of the framework. Due to the inherent multifunctionality of the material the configuration of the laminate can be alternated to provide suitable performance based on the purpose of the component.

2. The laminated structural battery composite

There are two proposed battery configurations of the structural battery composite, the laminated structural battery and the 3D structural battery. The laminated structural battery was first proposed by Wetzel et. al [2, 3] and later demonstrated by Ekstedt et al. [4] and Carlson [5]. The 3D structural battery was developed by Asp and co-workers [5-8] and a comprehensive review of the realization of structural battery composites and research done within the field has been provided by Asp and Greenhalgh [9]. In this study, only the laminated structural battery is considered. In the laminated structural battery concept, the battery cell consists of several laminae stacked on top of each other. Each lamina has a separate function and works as electrode, separator or collector, etc., within the battery cell. The laminated structural battery concept is illustrated in Fig. 1.

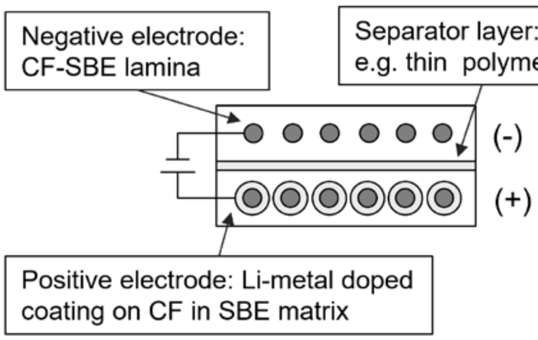

Figure 1. Illustration of the laminated structural battery concept.

In the schematic illustration of the laminated battery cell in Fig. 1, the upper lamina corresponds to the negative electrode of the battery cell. The negative electrode lamina consists of structural battery electrolyte (SBE) developed by Ihrner et al. [10], reinforced with PAN-based carbon fibres. The electrochemically active material is the carbon fibres. PAN-based carbon fibres have in previous studies [11-14] shown high electrochemical performance (here referring to capacity) similar to graphite used in commercially available Li-ion batteries. The lower lamina in the illustration corresponds to the positive electrode, which consists of coated carbon fibre reinforced SBE. The coating on the fibres is doped with lithium-metal-oxide based electrode material (e.g. $LiFePO_4$) which act as active positive electrode material. To avoid short-circuit, i.e. to ensure that the positive and negative electrodes do not come in contact with each other, a separator layer is needed between the two laminae. The separator layer needs to be electrically insulating (i.e. not conduct electrons) while allowing for transport of ions between the electrodes. The separator layer also needs to be thin to minimize ohmic losses and sufficiently stiff to prevent penetration and allow mechanical load transfer.

In addition to these components, the cell needs to be protected against moisture and have current collectors and connectors to connect the battery to an external circuit. One can also stack two or more cells on top of each other and by doing so construct different battery composite lay-ups.

3. Framework for assessing multifunctional performance

To estimate the multifunctional performance, i.e. the mechanical and electrical performance, of the structural battery composite a design framework has been developed. The derivation of the performance metrics related to mechanical and electrical performance are described in the following.

3.1. Mechanical performance

The mechanical performance is assessed estimating in-plane elastic properties of the composite laminate using Classical Laminate Theory (CLT). Under the assumption that the laminate is symmetric and balanced, i.e. no coupling between extension and bending, the laminate engineering constants can be defined as follows.

The stiffness matrix for the individual lamina with respect to the global coordinates of the laminate are defined as

$$[Q^*] = [T_\sigma]^{-1}\,[Q]\,[T_\varepsilon]. \tag{1}$$

In Eq. (1) $[T_\sigma]$ and $[T_\varepsilon]$ corresponds to the transformation matrices, used to transform the directional properties of the individual lamina to the global coordinates of the laminate. The stiffness matrix $[Q]$, defined with respect to the directional properties of the lamina, is based on the elastic properties of the individual lamina E_L, E_T, ν_L, ν_T and G_{LT}. These properties can be derived using micromechanical models or be based on experimental data. Due to the battery cell configuration of the structural battery composite the properties of each lamina will vary significantly depending on the considered layer.

The extensional stiffness matrix for the laminate is defined as

$$A_{ij} = \Sigma_k\,(Q_{ij}^*)_k\,(h_k - h_{k-1}), \tag{2}$$

where $(h_k - h_{k-1})$ represents the thickness of the k^{th} layer. Given the assumption of symmetric lay-up we can define the matrix:

$$[a^*] = t_l\,[A]^{-1}, \tag{3}$$

where t_l corresponds to the thickness of the laminate. The in-plane effective moduli can now be estimated as

$$E_x = 1 / a_{11}^*,$$
$$E_y = 1 / a_{22}^*, \tag{4}$$
$$G_{xy} = 1 / a_{66}^*.$$

The in-plane elastic properties of the laminate are defined with respect to the global coordinates of the laminate presented in Fig. 2 and depend on the properties of the individual laminae e.g. volume fraction of fibres, material properties of constituents, lamina thickness and fibre direction.

3.2. Electrical performance

The electrical performance is assessed by estimating the specific capacity and energy density of the full component. The battery capacity is obtained as the product of the current and time during discharge. The actual capacity varies e.g. with discharge rate (C-rate) and temperature and can be defined per gram, referred to as specific capacity. The energy density is derived by multiplying the specific capacity with the nominal voltage during discharge. The specific capacity and energy density refers to the amount of energy that can be stored in the material and is estimated as described below. It should be noted that the active materials within the battery cell do not need to be balanced. However, to improve the specific capacity and the energy density it is beneficial to have balanced amount of active materials.

The specific capacity C is defined as

$$C = \int I \, \mathrm{d}t \, / \, m, \tag{5}$$

where $\int I \, \mathrm{d}t$ is the definite integral of the electric current over the time for discharge and m is the mass of the electrochemical active material.

The capacities of the negative and positive electrodes in the laminated structural battery can be defined as

$$\begin{aligned} c_{\mathrm{neg}} &= C_{\mathrm{f}} \, A_{\mathrm{c}} \, \Sigma t_{\mathrm{neg}} \, V_{\mathrm{f,neg}} \, \rho_{\mathrm{f}}, \\ c_{\mathrm{pos}} &= C_{\mathrm{p}} \, A_{\mathrm{c}} \, \Sigma t_{\mathrm{pos}} \, V_{\mathrm{p,pos}} \, \rho_{\mathrm{p}}. \end{aligned} \tag{6}$$

In Eq. (6) C_{f} and C_{p} are the specific capacity of carbon fibres (subscript f) and $LiFePO_4$ particles (subscript p) respectively. The total area of the battery cells in the component is defined as A_{c} and the total thickness of the negative and positive electrodes in one of the cells are defined as Σt_{neg} and Σt_{pos}. The volume fraction of fibres in the negative lamina is defined as $V_{\mathrm{f,neg}}$ and the volume fraction of $LiFePO_4$ particles in the positive lamina is defined as $V_{\mathrm{p,pos}}$. The density of carbon fibres is defined as ρ_{f} and the density of $LiFePO_4$ particles is defined as ρ_{p}.

The specific capacity of the full component can now be estimated as

$$C_{\mathrm{C}} = \min(c_{\mathrm{neg}} \, , \, c_{\mathrm{pos}}) \, / \, w_{\mathrm{C}}, \tag{7}$$

where w_{C} is the total weight of the component, which can be derived using assumed lamina thicknesses, volume fractions and material densities. In the case of balanced amount of active materials, the difference in capacity of the electrodes is zero which results in higher specific capacity of the component.

The energy density can be estimated as

$$\Gamma_{\mathrm{C}} = V_{\mathrm{n}} \, C_{\mathrm{C}}, \tag{8}$$

where V_{n} is the nominal voltage during discharge. As can be seen from the derivations above the specific capacity and energy density is dependent on e.g. capacities of active materials, volume fractions, material densities and lamina thicknesses. This means that the specific capacity and energy density are directly linked to the elastic properties of the material as discussed in section 3.1.

4. Case study: Structural battery demonstrator

The considered demonstrator is made from 10 laminated battery cells connected in series between protective reinforcement plies. In this work the nominal cell voltage during discharge for each cell is assumed to be 2.8 V. This assumption is based on the active materials considered in this work (carbon fibres and $LiFePO_4$). Given a nominal cell voltage for each cell of 2.8 V, 10 cells in series will provide an output voltage of 28 V. The proposed layout of the demonstrator is schematically illustrated in Fig. 2.

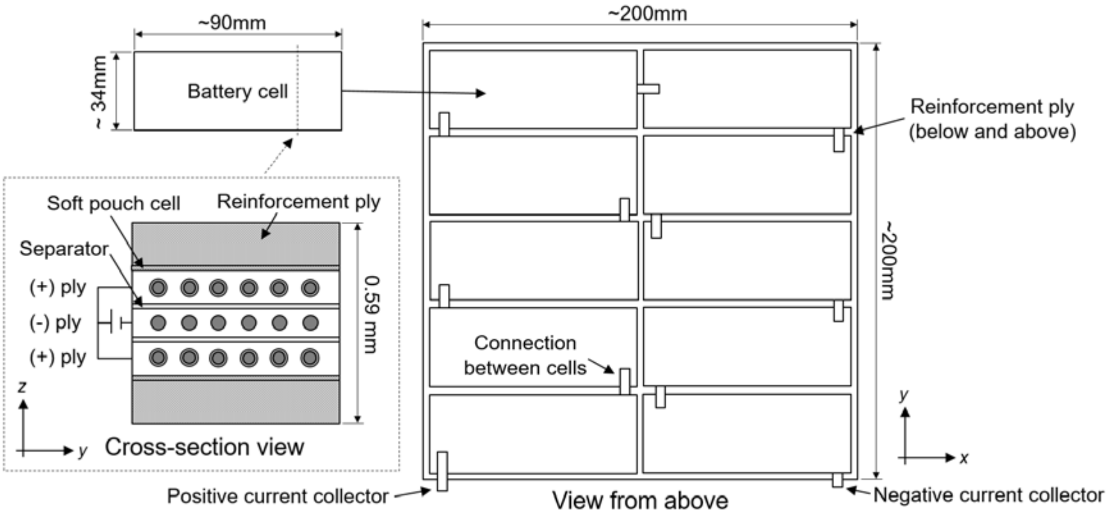

Figure 2. Concept description of demonstrator for which the developed design framework has been used to estimate its mechanical and electrical performance.

As can be seen in the cross-section view of the battery cell in Fig. 2, the cell concept used in the demonstrator is an extended version of the laminated battery cell described in section 2. The specific capacity of the positive electrode is assumed to be in the order of one half of the capacity of the negative electrode. This is based on experimental studies by Johannisson et al. [15] on negative lamina half-cells and work done on electrochemical properties of commercially available PAN-based fibres [10-13] as well as on ongoing research at KTH on electrophoretic deposition of LiFePO4 on carbon fibres. To balance the battery cell the electrode materials must be proportional to the provided capacity and for this reason, more positive electrode material is needed compared with negative electrode material. To improve the electrical performance related to power, the positive electrode lamina in Fig. 1 is split into two laminae to reduce the distance between the electrodes. The positive electrode laminae are placed above and below the negative electrode lamina as illustrated in the cross-section view in Fig. 2. This lay-up also ensures that the laminate is balanced and symmetric as the thicknesses of the electrode laminae are altered for the different configurations evaluated. The cells are protected against moisture by adding layers/laminae of soft pouch cell material, surrounding each cell. The cells are then placed on a reinforcement ply and connected in series before an additional reinforcement ply is placed on top of the cells. The cells are connected via copper and aluminium foil pieces and additional foil pieces are added at the lower corners of the demonstrator as current collectors. The reinforcement plies are made from woven fabric CRFP and in addition to providing a base layer for the battery cells to be placed on, the plies protect the cells and reinforce the structure.

Three laminate configurations have been chosen to illustrate the multifunctionality of the material and how the mechanical and electrical performance can be altered by modifying the cell configuration. For simplicity only the volume fraction of active materials (carbon fibres and $LiFePO_4$ particles) and thicknesses of electrode laminae are altered to enhance the mechanical and electrical performance respectively. The same total thickness of the complete laminate (590 µm) is used for all cases providing comparable stiffness measures. The number of plies, thickness, volume fraction of active electrode materials and fibre directions for the battery cells are presented in Table 1.

Table 1. Assumed properties for the individual plies of the battery cells illustrated in Fig. 2.

Lamina	Number of plies (-)	V_f (-)	$V_{p,pos}$ (-)	Thickness (µm)	Fibre direction (degrees)
Reinforcement ply	2	0.5	-	100	[0/90]
Soft pouch cell layer	2	-	-	30	-
Negative electrode	1	$V_{f,neg}$	-	t_{neg}	0
Separator	2	-	-	15	-
Positive electrode	2	$V_{f,pos}$	$V_{p,pos}$	t_{pos}	0

The volume fraction of fibres in the positive lamina $V_{f,pos}$ depends on the assumed volume fraction of $LiFePO_4$ particles $V_{p,pos}$. The volume fractions of active materials ($V_{f,neg}$ and $V_{p,pos}$) and thicknesses of electrode laminae (t_{neg} and t_{pos}) for the three evaluated cell configurations are presented in Table 2.

Table 2. Assumed volume fraction of active materials (carbon fibres and $LiFePO_4$ particles) and thicknesses of electrode laminae for the three evaluated cell configurations.

Configuration	Enhanced performance	Balanced/ unbalanced cell	$V_{f,neg}$ (-)	$V_{p,pos}$ (-)	t_{neg} (µm)	t_{pos} (µm)
A	Mechanical	Unbalanced	0.6	0.15	200	50
B	Electrical	Balanced	0.6	0.5	140	80
C	Intermediate	Unbalanced	0.5	0.35	200	50

Material densities and specific capacity of active electrode materials used to compute performance metrics for the demonstrator configurations are presented in Table 3.

Table 3. Material densities and specific capacity of the structural battery constituents.

Material	Density (g/cm^3)	Specific capacity (mAh/g)
Carbon fibre	1.8	200
$LiFePO_4$	3.6	100
Coating on fibres (positive lamina)	2.1	-
Polymer matrix (SBE)	1.1	-
Separator (porous PE)	0.53	-
Reinforcement plies	1.5	-
Soft pouch cell	2.0	-

In this analysis, it is assumed that the fibres of the electrode laminae are placed in the same direction. This assumption is made to simplify the manufacturing procedure of the battery cells and to ensure that the laminate is balanced and symmetric. Also, in the analysis of the elastic properties of the demonstrator, it is assumed that there is no gap between battery cells and the elastic properties of the individual lamina are approximated using Rule of mixture and Halpin-Tsai.

4.1. Multifunctional performance of the structural battery demonstrator

The performance metrics for the three configurations of the demonstrator are derived using the developed framework. The results are presented in Table 4.

Table 4. Performance metrics for the three configurations of the demonstrator.

Configuration	E_x (GPa)	E_y (GPa)	G_{xy} (GPa)	C_C (mAh/g)	Γ_C (Wh/kg)	w_C (g)
A	89.1	14.2	1.23	19.4	54.4	36.9
B	52.6	13.6	1.11	34.8	97.4	42.0
C	68.4	13.8	1.14	28.3	79.3	37.8

As indicated by the performance metrics derived for the different configurations, presented in Table 4, it is possible to alter the design in order to provide suitable performance based on the purpose of the component. To illustrate this, the energy density of the demonstrator is plotted against the shear modulus for the three configurations in Fig. 3.

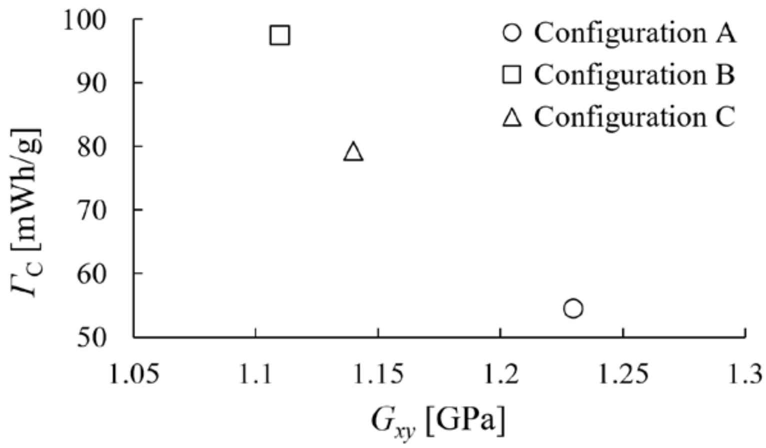

Figure 3. The energy density plotted against the shear modulus for the three configurations.

As can be seen in Fig. 3, configuration A has a higher shear stiffness while providing a lower energy storage capability. By minor modifications in the laminate configuration, the energy density can be significantly improved but with a cost of a reduced stiffness and a slight increase in mass, as in the case of configuration B. This mass penalty is related to the amount of positive active material.

5. Conclusions

In this study a novel framework to estimate the mechanical and electrical performance of laminated structural battery composites has been developed. Multifunctional performance metrics are derived for three laminate configurations of a structural battery composite demonstrator utilizing the developed framework. The results indicate that with minor modifications in the laminate configuration, the mechanical and electrical performance of the composite laminate can be altered. This means that the performance of the material can be adapted to provide suitable properties based on the requirements on the component. The results also demonstrate the capabilities of the framework and illustrate the multifunctionality of the material.

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