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A residual performance methodology to evaluate multifunctional systems

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Abstract

The development of multifunctional materials and structures is receiving increasing interest for many applications and industries; it is a promising way to increase system-wide efficiency and improve the ability to meet environmental targets. However, quantifying the advantages of a multifunctional solution over monofunctional systems can be challenging. One approach is to calculate a reduction in mass, volume or other penalty function. Another approach is to use a multifunctional efficiency metric. However, either approach can lead to results that are unfamiliar or difficult to interpret and implement for an audience without a multifunctional materials or structures background.

Instead, we introduce a comparative metric for multifunctional materials that correlates with familiar design parameters for monofunctional materials. This metric allows the potential benefits of the multifunctional system to be understood easily without needing a holistic viewpoint. The analysis is applied to two different examples of multifunctional systems; a structural battery and a structural supercapacitor, demonstrating the methodology and its potential for state-of-the-art structural power materials to offer a weight saving over conventional systems. This metric offers a new way to communicate research on structural power which could help identify and prioritise future research.

1. Introduction

There is a growing interest in adopting multifunctionality to produce more efficient and environmentally-friendly materials and structures to address the challenges of lightweighting and energy storage [1]. For instance, NASA regards multifunctionality as a critical attribute for future deep space missions [2]. Multifunctionality is achieved by combining one or more, conventionally disparate, functions into a single material or structure [3], which can include load carrying, structural health monitoring, morphing, self-healing, energy storage, etc [4, 5]. Fibre composite materials are a particularly attractive platform for developing multifunctional systems, as they already deliver excellent mechanical performance whilst offering considerable versatility in composition and microstructure. Furthermore, the relatively benign fabrication conditions for carbon fibre reinforced polymer (CFRP) composites (moderate temperatures and pressures) permits the incorporation of processing-sensitive functions. Introducing functions beyond structural load bearing can be achieved with or without modifying the constituents of the composite material [6], however, this typically results in some compromise in the structural performance. In *multifunctional materials* [7], the constituents (e.g. fibres, matrices, etc) undertake more than one function throughout the whole material, whilst in *multifunctional structures*, the multiple functions are provided by distinct monofunctional materials which have been assembled together. Carbon fibre reinforced polymer composites are particularly appropriate choices for multifunctional applications [8], because the carbon fibres offer both attractive mechanical and electrical properties [9]. One class of multifunctional material which is currently receiving considerable attention is structural power composites [10], which store electrochemical energy within the composite component: various devices have been fabricated, including structural batteries [11], structural capacitors [12], structural supercapacitors [13] and structural fuel cells [14]. Structural power composites typically contain a structural electrolyte which needs to satisfy two contrasting requirements: high ionic conductivity for good electrochemical performance and high elastic modulus for good mechanical performance.

1.1. Structural batteries

Structural batteries use the same lithium-ion battery technology as their conventional monofunctional counterparts: two electrodes, the cathode (positive electrode) and the anode (negative electrode), and a separator layer placed in an ion-conducting electrolyte. When current is applied and the battery charges, lithium ions shuttle from the cathode to the anode, creating an electrical potential difference between the electrodes. The opposite reactions enable the battery to deliver electrical power. First developed in a structural form by the US Army Research Laboratory [15], researchers have taken different approaches to exploit this technology. The first, laminated structural batteries (LSB), are effectively fibre-matrix laminates, in which each layer is designed for both electrochemical and mechanical properties [16]. Carbon fibres are used as electrodes for their excellent load carrying capability and good lithium ion intercalation properties, which is essential for efficient battery design [17]. While in conventional batteries a liquid electrolyte is used, LSBs require a solid electrolyte to maintain rigidity and load-carrying capability. A structural battery electrolyte (SBE) [18] based on a two-phase percolating network has been developed, which allows ionic redox reactions to take place while ensuring structural rigidity. Research has also been targeted towards improving the performance of the anode, with silicon-coated carbon nanotubes presenting a 2.5 times higher specific capacity than previous anodes [19].

In parallel, a different approach to making structural batteries has also been developed [20]: instead of using laminates of carbon fibres as electrodes, they use individual fibres. By depositing the cathode and electrolyte onto the carbon fibre and encapsulating the coated fibres in a multifunctional matrix, a 3D structural battery was created.

1.2. Structural supercapacitors

Supercapacitors are appropriate electrochemical energy storage devices when high power and high cyclability are required. Unlike batteries, supercapacitors harness electrical energy from electrostatics. Two high surface area electrodes are separated by an ionically-conducting but electrically-insulating separator all soaked in an electrolyte. The accumulated charge at the interface between each electrode and the electrolyte stores the electrical energy. Structural supercapacitors operate in the same manner whilst also providing mechanical load carrying capabilities. A structural supercapacitor has been developed using two woven carbon fibre electrodes in a multifunctional matrix, separated by a woven glass fibre separator [21]. Increasing the surface area of the electrodes results in a higher capacitance [22]. Carbon aerogel modified electrodes have been used to greatly increase the surface area of the electrodes and yield specific power values up to 1.2 kW kg^{-1} [23]. However, their specific energy, around 1 Wh kg^{-1}, remains lower than that of conventional supercapacitors and the cell working voltage is limited by the electrolyte breakdown voltage, which is typically around 2.7 V [24].

1.3. Multifunctional efficiency and performance metrics

For multifunctional materials or structures to be advantageous compared to conventional, compartmentalised, monofunctional constituents, they need to demonstrate an improvement in, for instance, overall system mass, volume or cost. A common metric to rank the performance of multifunctional systems in comparison to monofunctional systems is through a single metric called the multifunctional efficiency index: $\eta_{mf} = \eta_s + \eta_d$, where η_s and η_d are the structural and device efficiencies (i.e. multifunctional performance divided by monofunctional performance [25–27]). If η_{mf} exceeds unity, the multifunctional material offers a mass or volume saving over the conventional monofunctional system. A more complex analysis methodology for multifunctional composites is a material-architecture index [28], which has been applied to structural battery laminate designs. This method involves eight steps similar to those used for typical design optimisation problems to derive the indices for stiffness and strength-limited designs at minimum weight. This methodology is limited to symmetric composite beams with uniform cross-sections and materials. However, one difficulty with applying such metrics is that few publications provide enough data to fully compare multifunctional with monofunctional system properties.

To enable engineers to decide how well a multifunctional material can perform for a given application, there is a need for a more robust comparative methodology. One major challenge for a multifunctional material is that a single separate function alone will never outperform a corresponding state-of-the-art monofunctional material or device. Hence, if only considering a single function (such as bending deflection) of a multifunctional system, the gain of the multifunctional system can easily be overlooked. To address this challenge, we present a new metric to permit a holistic comparison of the properties in multifunctional systems against the equivalent monofunctional reference properties. The approach is to project the properties from the multifunctional design space to the monofunctional parameter space by normalizing by the additional material requirement, rather than the total quantity of material. The resulting residual specific properties for the multifunctional material can be compared to specific properties of the monofunctional systems.

The residual specific properties are demonstrated using two application examples; a structural battery and a structural supercapacitor using current state-of-the-art performance data for commercial devices and projected performance data for the multifunctional systems. These examples show how the methodology can be implemented, and the resulting residual specific properties indicate how structural power composites can potentially outperform equivalent monofunctional systems.

2. Methodology

The methodology herein is described for a system which has some defined requirements for electrical properties and mechanical properties. The best monofunctional solution, which can satisfy these requirements and minimize a penalty-parameter that depends on the desired outcome of the design process is considered known. Traditionally, mass is used for transport applications, whereas volume may be more important for consumer electronics. Herein, we will for simplicity consider mass saving, though the methodology is the same for any penalty-parameter. Traditionally, system mass savings are made by decreasing the mass of the sub-systems independently, e.g. the mass of a battery pack and the mass of the load-carrying structure. Alternatively, a multifunctional design can be considered which also satisfies the same system requirements. The multifunctional design combines the electrical and mechanical properties into the same material or structure as shown in figure 1.

For the monofunctional electrical sub-system, it has given electrical requirements of energy w and power p. To decrease the mass, a screening is made of different solutions and an optimal selection with the highest specific properties $\bar{w}$ and $\bar{p}$ is chosen, since it reaches the lowest electrical sub-system mass m_1 given by:

$$m_1 = \max\left(\frac{w}{\bar{w}}, \frac{p}{\bar{p}}\right). \tag{1}$$

Similarly, the monofunctional structural sub-system can have many different requirements, including stiffnesses and strengths. These could include limitations on bending deflection z, in-plane stiffness A_x, shear strength τ_{xy}, etc. The optimal solution for maximizing the mass saving then has the best corresponding specific properties $\bar{z}$, $\bar{A}_x$, $\bar{\tau}_{xy}$, providing a structural sub-system mass m_2 as:

$$m_2 = \max\left(\frac{z}{\bar{z}}, \frac{A_x}{\bar{A}_x}, \frac{\tau_{xy}}{\bar{\tau}_{xy}}\right). \tag{2}$$

Often, the design of a system stops here, since a lowest possible system mass $(m_1 + m_2)$ has been reached. Any further design considerations would follow the same procedure, possibly finding a solution with better specific properties which incrementally reduces the mass of that sub-system.

Alternatively, a multifunctional material can be used to fulfil all the requirements w, p, z etc. Traditionally, if such a multifunctional material is included in the design choices above, its specific properties are calculated by $\bar{w}_{mf} = \frac{w}{m_{mf}}$, $\bar{p}_{mf} = \frac{p}{m_{mf}}$, $\bar{z}_{mf} = \frac{z}{m_{mf}}$ and so on, where m_{mf} is the total mass of the multifunctional material. The challenge with multifunctionality in this case is that any multifunctional material can never have a larger $\bar{w}_{mf}$ than $\bar{w}$ or $\bar{p}_{mf}$ than $\bar{p}$, etc. and thus will always be considered inferior to monofunctional solutions and rejected. This is because the addition of a new function will invariably add some mass to the multifunctional system, and so there are lower bounds on the multifunctional system mass as given in equation (3).

$$m_{mf} > m_2 \text{ and } m_{mf} > m_1. \tag{3}$$

These lower limits are directly linked to the quality and performance of the systems that are being compared: i.e. it is not possible to compare a high-performance multifunctional system with low performance monofunctional systems.

We now present two relative masses to be considered when comparing a multifunctional system with two monofunctional sub-systems. These *residual masses* are the differences in mass between the multifunctional

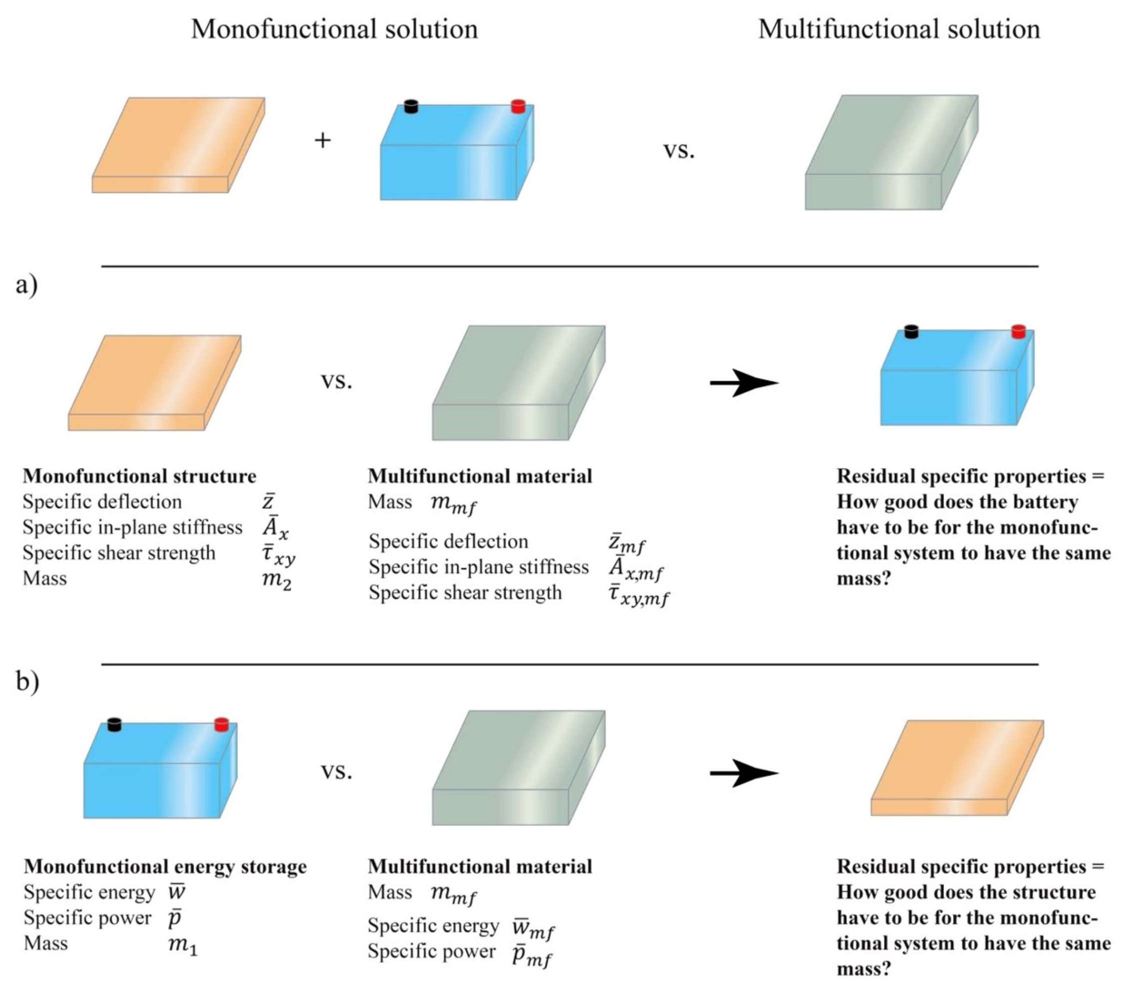

Figure 1. Diagram showing the comparison between two monofunctional systems versus a multifunctional system. One way to present the residual specific properties is by separating the comparisons into: (a) a monofunctional structure is compared to a multifunctional solution. The mass difference between the two is the residual mass for the monofunctional battery, and the residual specific properties are essentially how good the monofunctional battery has to be in order for the monofunctional solution to have the same properties as the multifunctional. (b) A monofunctional battery is compared to a multifunctional solution. The mass difference between the two is the residual mass for the monofunctional structure, and the residual specific properties are essentially how good the monofunctional structure has to be in order for the monofunctional solution to have the same properties as the multifunctional.

system and the corresponding monofunctional sub-systems providing equal functional performance and are given as:

$$m_{res,1} = m_{mf} - m_2 \tag{4}$$

$$m_{res,2} = m_{mf} - m_1. \tag{5}$$

Essentially, $m_{res,2}$ is the surplus mass for the monofunctional energy-storing system, such that the monofunctional sub-systems have the same total mass as the multifunctional system (figure 1(a)), and similarly $m_{res,1}$ is the surplus mass for the monofunctional structural system, such that the monofunctional sub-systems have the same total mass as the multifunctional system (figure 1(b)). The multifunctional residual specific properties are then calculated as:

$$\bar{w}_{res} = \frac{w}{m_{res,i}},\ \bar{p}_{res} = \frac{p}{m_{res,i}},\ \bar{z}_{res} = \frac{z}{m_{res,i}},\ etc \tag{6}$$

where $m_{res,i}$ $(i = \text{parameter 1},\ \text{parameter 2})$ is defined as the residual mass of function i in the multifunctional system and the parameter number specifies the multifunctional aspect begin considered.

Utilizing these residual specific properties in the design choices for the systems above could highlight the benefits from incorporating a multifunctional material and allow direct comparisons to be made with the traditional monofunctional design parameters for monofunctional sub-systems. Essentially, this

Table 1. Data for a structural battery, a CFRP panel and a lithium ion battery given from [29].

System demands	Monofunctional data		Multifunctional data	
Midpoint deflection limit z	Total mass m	3.54 kg	Structural battery mass	2.64 kg
0.65 mm	Structure mass m_2	1.87 kg	Residual structure mass $m_{res,2}$	0.97 kg
Total energy w	Battery mass m_1	1.67 kg	Residual battery mass $m_{res,1}$	0.77 kg
286 Wh	Battery specific energy $\bar{w}$	171 Wh kg^{-1}	Residual specific energy $\bar{w}_{res}$	371 Wh kg^{-1}
			Multifunctional efficiency index η_{mf}	1.26

methodology identifies what specific performance level the monofunctional components would need to achieve to match the weight saving of a multifunctional system. If the monofunctional component performance levels are below the residual specific values identified, the multifunctional system represents a preferable holistic design solution.

3. Examples

As a demonstration, the methodology presented in Section 2 it has been applied to two structural energy storage materials: a structural battery and a structural supercapacitor. The results from these examples are also evaluated using the multifunctional efficiency index approach as presented by Snyder *et al* [25].

3.1. Structural battery

Consider an example system that requires an energy w of 286 Wh and can simultaneously support a uniformly distributed pressure of 1 N m^{-2} (as presented in [29]) with minimal deflection for a given system mass. In this example, other requirements such as power or strength are not considered because structural battery data for these properties have not yet been determined.

An optimised *monofunctional* system could contain an electrical sub-system (mass $m_1 \approx 1.67$ kg) made from standard Li-ion batteries with a specific energy $\bar{w}$ of 171 Wh kg^{-1} [29]. The structural sub-system could be a 1 m $\times$ 1 m $\times$ 1 mm simply-supported CFRP panel [29]. This panel is made from unidirectional epoxy prepreg with a quasi-isotropic (QI) lay-up ($[0, 90, -45, 45]_s$) and $m_2 \approx 1.87$ kg [29]. Excluding the panel's self-weight, the midpoint bending deflection z under this pressure loading would be 0.65 mm.

Now consider an optimised *multifunctional* structural battery composite panel with the same area and QI lay-up capable of storing the same required energy (286 Wh) [29]. For this structural battery panel to not exceed the midpoint deflection limit reached by the CFRP panel under the same 1 N m^{-2} load case, the thickness of the structural battery panel needs to be 1.4 mm [29]. This structural battery that can match the monofunctional energy requirement and deflection limit (w and z) has a total mass of about 2.64 kg. Thus, the residual analysis for this structural battery yields a residual specific energy $\bar{w}_{res}$ of 371 Wh kg^{-1} (table 1), and a multifunctional efficiency index [25] of 1.26.

An insight into interpreting the values in table 1 is the following: by utilizing a 2.64 kg structural battery, and comparing this to a 1.87 kg monofunctional structure, the 0.77 kg residual mass (according to equation (4)) of the structural battery is the equivalent 'energy storing' constituent of the whole system. Thus, a monofunctional battery containing the same amount of energy would need a specific energy of 286 Wh/0.77 kg = 371 Wh kg^{-1} (equation (6)).

3.2. Structural supercapacitor

For the purpose of demonstrating the applicability of the residual analysis method, here we consider a slightly different design scenario and assume that equation (1) leads to two functions being the limiting properties: electrochemical power and midpoint bending deflection. This example system needs a power p of 2.80 kW and must also support a uniformly distributed pressure of 1 N m^{-2} with minimal deflection.

An optimised *monofunctional* system could contain an electrical sub-system (mass $m_1 = 0.68$ kg) made from state-of-the-art commercial supercapacitors with a specific power $\bar{p}$ of 4.10 kW kg^{-1} [30]. The structural sub-system is the same 1 m $\times$ 1 m $\times$ 1 mm simply-supported CFRP panel described in the structural battery example ($m_2 = 1.90$ kg) [29].

Now consider an optimised *multifunctional* structural supercapacitor [31] panel with the same area and capable of delivering the same required power (2.80 kW). For this structural supercapacitor panel to not exceed the midpoint deflection limit reached by the CFRP panel under the same 1 N m^{-2} load case, the mass of the structural supercapacitor panel needs to be 2.55 kg. Thus, the residual analysis for this structural supercapacitor yields a residual specific power $\bar{p}_{res} = 4.33$ kW kg^{-1} (table 2) whilst the multifunctional efficiency index [25] is 1.01.

Table 2. Structural supercapacitor [31], CFRP panel and Maxwell 150 F supercapacitors [30] data.

System demands	Monofunctional data		Multifunctional data	
Midpoint deflection limit z	Total mass m	2.58 kg	Structural supercapacitor mass	2.55 kg
0.65 mm	Structure mass m_2	1.90 kg	Residual structure mass $m_{res,2}$	1.87 kg
Total power p	Supercapacitor mass m_1	0.68 kg	Residual supercapacitor mass $m_{res,1}$	0.65 kg
2.80 kW	Supercapacitor specific power $\bar{p}$	4.10 kW kg^{-1}	Residual specific power $\bar{p}_{res}$	4.33 kW kg^{-1}
			Multifunctional efficiency index η_{mf}	1.01

The data in table 2 can be interpreted as using a 2.55 kg structural supercapacitor compared to a 1.90 kg monofunctional structure yields a residual mass of 0.65 kg according to equation (4). Thus, a monofunctional supercapacitor must have a specific power (equation (6)) of 2.80 kW/0.65 kg = 4.33 kW kg^{-1} for the combined monofunctional components to have equal mass to the structural supercapacitor. Conversely, a structural supercapacitor of 2.55 kg compared to 0.68 kg of monofunctional supercapacitors leaves 1.87 kg residual mass (equation (5)). The residual specific power slightly exceeds the monofunctional specific power. This comparison indicated that the state-of-the-art structural supercapacitor merits consideration as a potential solution. Further analysis may be performed to investigate other benefits achievable from using the multifunctional system, such as potential safety improvements from having a distributed rather than concentrated energy source.

4. Discussion and conclusion

This paper introduces a new methodology to compare residual specific properties of a multifunctional system to well-known conventional specific properties of monofunctional sub-systems. The residual specific properties are based on a residual mass, which is the difference in mass between the multifunctional system and the corresponding monofunctional component mass. The methodology computes the required performance of selected monofunctional components so that the combined mass of the monofunctional components is the same as that of the multifunctional material system.

This approach has an advantage over other multifunctional efficiency metrics [25–27] in that it provides values that are already familiar to engineers or scientists working in the respective fields. Besides, this residual metric can be directly compared in a screening of different material or energy/power storage options and does not require a holistic system viewpoint to be understood. This metric could also be expanded to evaluate potential volume or cost savings instead of mass, or one can incorporate other properties for comparing with monofunctional materials, structures or systems.

The residual specific properties presented in this paper has an inherent limitation, it cannot compare the systems if the mass of the multifunctional system is smaller than any of the monofunctional systems. This constraint is inherently fulfilled, since a material will almost certainly gain mass with added functions. But it imposes a restraint on the comparative monofunctional systems; they need to be of similar performance.

To gain a complete understanding of the performance enhancements provided by a multifunctional system, it is essential to have baseline monofunctional performance data with which to compare against. However, publications in this field presenting new multifunctional systems often lack this corresponding benchmark monofunctional data. Therefore, we recommend that future studies on new multifunctional systems (both multifunctional materials and multifunctional structures) would benefit from being accompanied by equivalent monofunctional performance results and the key limiting material properties for a given component/application corresponding to both functions. This complete data set would enable researchers in the field to accurately quantify and evaluate the relative improvements offered by the multifunctional system, facilitate progress in this field and potentially promote adoption of the new multifunctional system.

The residual specific metric presented here offers a new perspective on multifunctionality; it relates multifunctional performance parameters to common monofunctional performance parameters. This residual perspective can help to disseminate and emphasize the considerable potential of multifunctional materials, which could help identify needs for future research in the field.

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