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DESIGN OF OPTIMISED MULTI-SCALE STRUCTURES FOR MULTIFUNCTIONAL COMPOSITES

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Abstract

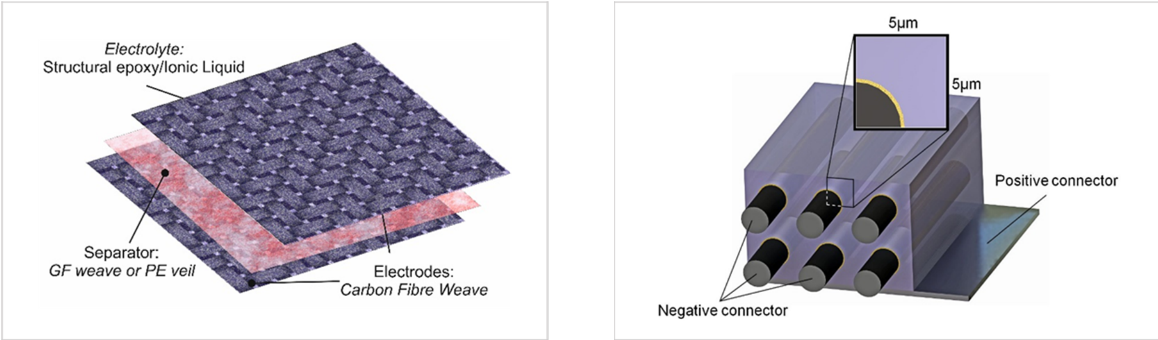
The multi-scale structures are commonly found in nature, such as plants and bones. Such multi-scale structures can be divided into macro-scale, micro-scale and further sub-scale structures. In this study, we aim to design optimised two-scale structures for multifunctional composites, specifically by enhancing the structural stiffness and the ionic conductivity simultaneously. To tackle this problem, a novel strategy for achieving optimised multi-scale structures is presented. A database of optimised micro-scale structures and simple placement criterion for the micro-scale structure were applied. We demonstrate the efficiency of our strategy by designing, optimising and evaluating two-scale structures composed of macro-and micro-scales. The advantage of our strategy for optimised multi-scale structures is presented and discussed by comparing the structural stiffness and the ionic conductivity of several two-scale structures composed of different microstructures such as the solid-void, uniform and varied microstructures.

1 Introduction

The study of multifunctional composites (MFCs) has attracted great attention over the last decade. Beyond the high specific strength and modulus of conventional composites, such MFCs add unique functions such as high thermal and electrical conductivity or even electrical energy storage capabilities [1–3]. Among the variant of MFCs, structural power composites can provide a load-bearing functionality (i.e. structural function) and store electrical energy (i.e. electrochemical energy storage function such as in supercapacitors) simultaneously. Such composites are very promising because they have a potential to replace conventional structural materials on various platforms such as electrical vehicles (EVs), unmanned aerial vehicles (UAVs) and other transportation, offering significant weight and volume savings. For example, Figure. 1 shows the proposed configurations of a composite battery and a composite supercapacitor from previous research [4,5].

Recent research has been focused on the architectures and constituents of devices such as batteries and supercapacitors, and material functionalization of structural polymer electrolytes (SPEs))[1–3]. As can be seen from Figure. 2(a), the SEM image of an SPE shows complex and porous micro-scale structures within the macro-architecture of devices. In addition, previous studies have shown that there is a trade-off between mechanical and electrochemical performance of SPEs. Hence, in this study, we focused on an efficient structural optimisation method to obtain the optimised multi-scale structures (MSSs) with high ionic conductivity and high structural stiffness.

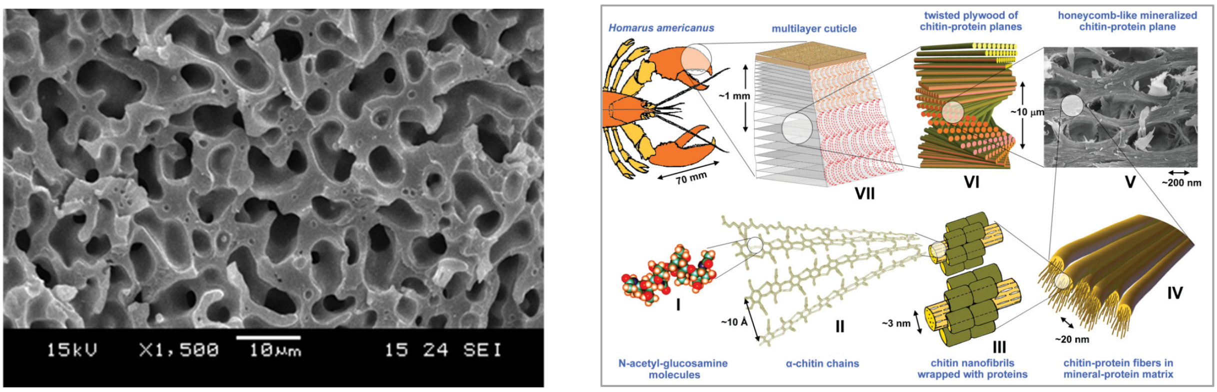
The MSSs are commonly found in nature, such as plants and bones, which can be divided into macro-scale, micro-scale and further sub-scale structures [6,7]. As can be seen from Figure. 2 (b), the diversity in sub-scale structures contributes to the bulk mechanical and multifunctional characteristics of final MSSs such as variable stiffness and strength, toughness, and thermal and electrical conductivity.



(a) Structural supercapacitor capacitor [4]

(b) Structural battery [5]

Figure. 1 Structural power systems; (a) structural supercapacitor and (b) structural battery



(a) SEM image of an epoxy-based SPE [4]

(b) Multi-scale structure of Lobster cuticle [8]

Figure. 2 Multi-scale structures in SPEs (a) and (b) Lobster cuticle

In most of the previous studies, the properties of the optimised macro-scale design were derived from the effective material parameters of a microstructure based on a homogenisation method in the structural analysis. A continuously distributed uniform micro-scale structure (MSS) was generally used to enhance manufacturability and reduce material costs [9,10]. However, a MSS with a uniform microstructure may be not optimal for more general loading scenarios. Moreover, it should be noted that although the homogenisation method uses effective material properties, it cannot reflect the effect of scales and configurations of real structures [11].

In our early work [12], a novel design methodology was proposed to achieve the optimised micro-scale structures for multifunctional polymer matrices, whereby a database of optimised microstructures under various loading conditions has been obtained by using a density-based topology optimization method (TO). These optimised microstructures constructed the finite element model-based database, which was utilised as the unit-cell models of MSSs. By introducing this database, considerable savings in computation cost of MSSs were provided.

In this study, we aimed to achieve multi-functional two-scale microstructures which have both high stiffness and high ionic conductivity for SPCs. To tackle this problem, we have utilised two inter-linked design mesh domains. Subsequently, a three-step process was applied to configure the optimised MSS. The novelty of the optimised MSSs is demonstrated and discussed by comparing the multifunctionality of various MSSs to the traditional continuous structure (i.e. single-scale). This paper culminates in the conclusions and future perspectives of this work.

2 Methodology

2.1 Multifunctionality; stiffness and ionic conductivity

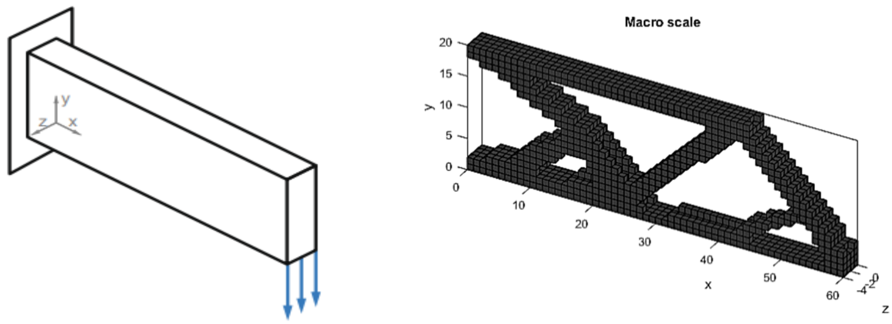
The multi-scale configuration of multifunctional matrix polymers (i.e. SPEs) is of interest in this study, which are required to provide both high stiffness and high ionic conductivity. Hence, the stiffness and the ionic conductivity were selected as performance indices to achieve the optimised MSSs. In particular, compliance was used to evaluate the stiffness of the MSS using the finite element method (FEM). Some studies have been performed to calculate the ionic conductivity in micro-scale by using FEM. However, they required significant computational effort to consider the complex effect of ion migration. Hence, a resistance network (RESNET) model [13] was employed here to evaluate the ionic conductivity of the MSSs with a reasonable computation effort.

2.2 Two-scale structures

In this study, two-scale structures were considered as a simple example of MSSs for SPEs; first, the optimised topologies of macro-scale structures were determined under given loading conditions by using a density-based TO. Subsequently, the optimised micro-scale structures placed into the macro-scale structure by replacing the unit cells based on three different placement criteria.

2.2.1 Optimised topology of the macro-scale structure

The optimised topology of the macro-scale structure was determined to maximize the structural stiffness (i.e. the minimization of compliance) by using TO [14]. The main function of macro-scale structures in this work is to provide high structural stiffness under given loading conditions. For instance, the optimised topology of a cantilever beam is presented as shown in Figure. 3. Hence, this optimised topology of the cantilever beam (see Figure. 3 (b)) can be utilised as a macro-scale structure for MSSs.



(a) Design domain (b) Optimised topology

Figure. 3 Topology optimization of 3D cantilever beam; (a) design domain and (b) optimised topology

2.2.2 Selection of the micro-scale structure

The pre-computed database of optimised micro-scale structures and simple placement criterion of the micro-scale structure were applied. In this study, a cubic design domain of voxels was utilized to obtain the optimised topology of micro-scale structures. We considered three separate cases in the design of MSSs to explore the multifunctionality with the varied placement of micro-scale structures; firstly, a fully solid and void element, where simply solid and void cubes were placed over the entire macro-scale domain. Secondly, a uniform micro-scale structure, with a uniform micro-scale structure for the macro-scale domain. Finally, a varied micro-scale structure, where type and direction of micro-scale structures were varied at each element of the macro-scale domain. Based on the dominant stress values of each element in the macro-scale mesh domain, the optimised microstructures replaced the element in the macro-scale mesh domain as shown in Figure. 4.

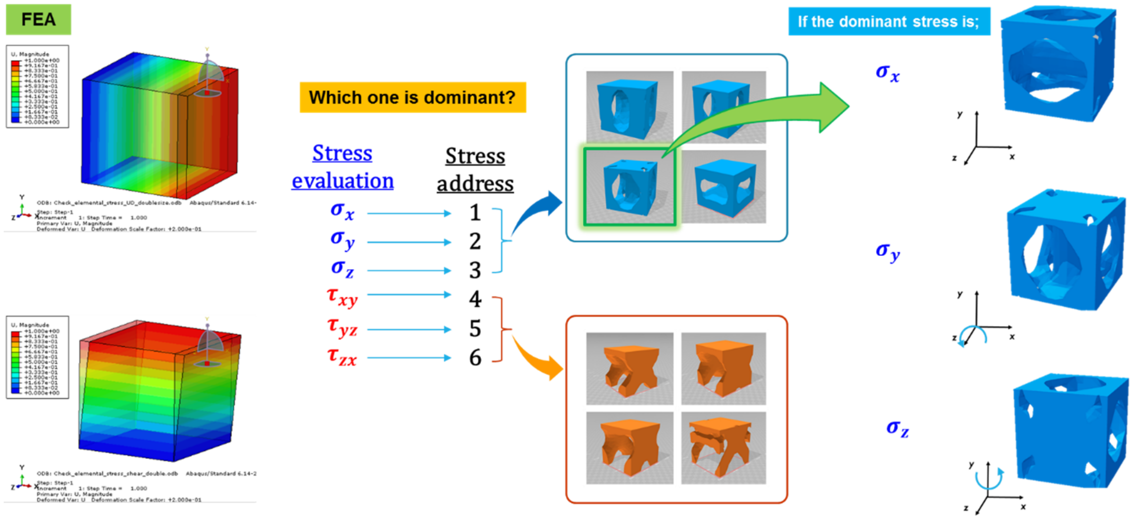


Figure. 4 Selection of optimised microstructures by evaluating a dominant elemental stress

2.2.3 MSS Configurations

MSSs were constructed with a macro-scale structure and multiple macro-scale structures. Hence, the mesh dimension of MSSs should be equivalent to the product of the macro-and micro-scale mesh dimensions. By a similar manner, the resultant volume fraction (or density fraction) of MSSs should be equivalent to the product of the macro-and micro-scale volume fraction (or density fraction) as shown in Figure. 5 [11]. As can be expected from this density relation, a number of combinations of MSSs with the same resultant density is available by adopting different macro-and micro-scale. Hence, MSSs having a similar volume fraction (or density fraction) were considered to compare the multifunctionality.

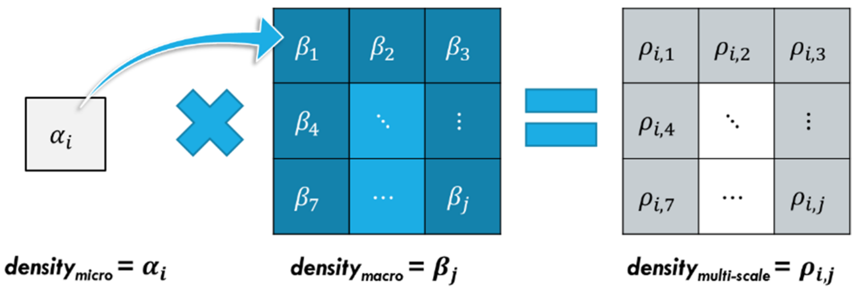


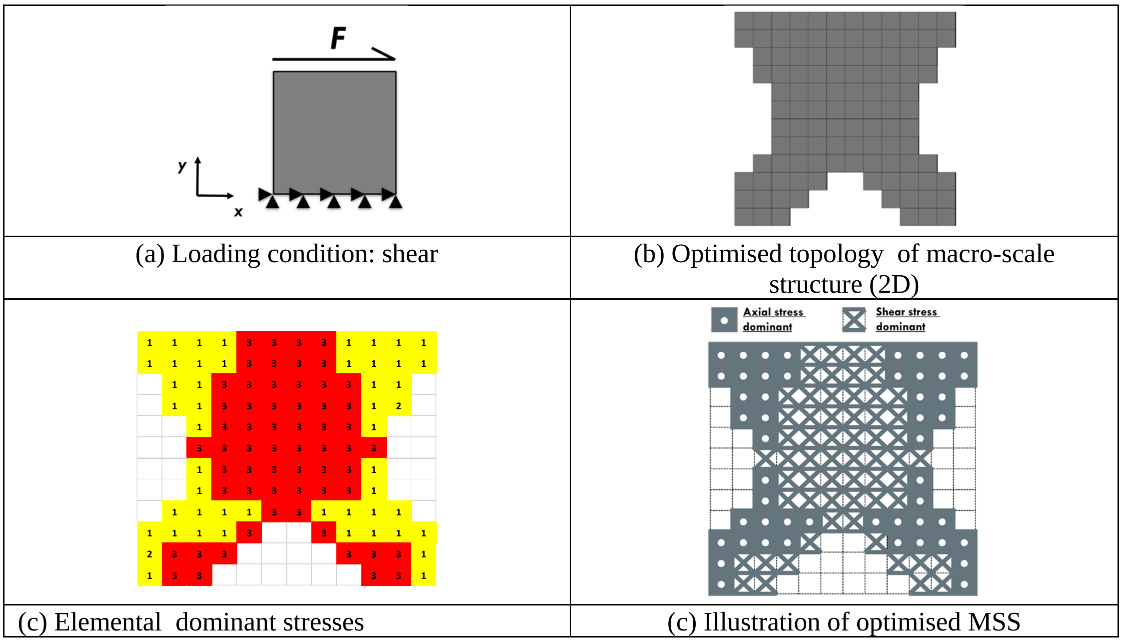
Figure. 5 Density relation between the multi-scale structure and the macro-and micro-scale structures

4 Results and discussion

4.1 Validation of selection criterion for micro-scale structures

To validate the selection criterion for micro-scale structures, a simple numerical simulation was performed as shown in Figure. 6. First, the optimised topology of the macro-scale structure under shear load was obtained in the 2D design domain (See Figure. 6 (a), (b)). Subsequently, the dominant stress of each element was evaluated

(See Figure. 6 (c)). As desired, the results of the elemental stress evaluation clearly presented the dominant stress and its direction of each element. Lastly, the optimised microstructures were placed into the corresponding elements based on the elemental stress evaluation results (See Figure. 6 (d)). This result successfully demonstrated the validity of the proposed selection criterion of micro-scale structures to achieve the optimised MSSs in this work.



(a) Loading condition: shear

(b) Optimised topology of macro-scale structure (2D)

(c) Elemental dominant stresses

(c) Illustration of optimised MSS

Figure. 6 Validation of selection criterion for micro-scale structures with a 2D example

4.2 Extension to 3D design domain; Uniaxial loading

As an extension of the application, 3D design domain was considered to validate the proposed design strategy for the optimised MSSs. To reassure the robustness and stability of the proposed strategy, we compared the simple 3D FEA results of our program, which was implemented in MATLAB code, with that of ABAQUS.

To explore and evaluate the multifunctionality of MSSs, five different structures were constructed under uniaxial loading with the same density fraction (d_f) as shown in Figure. 7; for these MSSs, the mesh dimension of 6×6×6 was used both for the macro-and micro-scale structures. Hence, the dimension of MSSs was constant as 36×36×36. Although, this dimension is not fully enough to satisfy the mesh convergence, it was selected as the simplest case for MSSs due to the limited computational capacity of normal workstations.

Among the five different structures, the Opt_Solid_L (see Figure. 7 (a)) represents the optimised topology with pure solid and void micro-scale structures from the low mesh resolution (i.e. 6×6×6). The next three cases of MSS_1, MSS_2 and MSS_3 (see Figure. 7 (b), (c) and (d)) illustrate the MSSs, which has a different combination of macro-and micro-scale structures. Lastly, the Opt_Solid_H (see Figure. 7 (e)) indicates the optimised topology with pure solid and void micro-scale structures from the high mesh resolution (i.e. 36×36×36). Hence, the Opt_Solid_H represents the optimal topology with the maximised stiffness corresponding the dimension of 36×36×36.

Figure. 8 presents the comparison of multifunctionality (i.e. stiffness and ionic conductivity) for five different multi-scale structures with uniform micro-scale structures (with a dimension of 36×36×36). As can be expected, the Opt_Solid_H showed the greatest structural stiffness because this case represents the real optimal topology under tension based on the dimension of 36×36×36, while Opt_Solid_H showed the lowest structural stiffness. Interestingly, the multifunctionality of the three MSSs (see Figure. 7 (b), (c) and (d)) showed relatively high stiffness and high ionic conductivity. The stiffness of MSS_1 was approximately 90% of maximised stiffness of the Opt_Solid_H. The ionic conductivities of the three MSSs were even higher than those of the Opt_Solid_L and the Opt_Solid_H. Importantly, the ionic conductivity of MSS_3 was approximately 130% greater than that of the Opt_Solid_H. As can be seen from these results, the MSSs are very promising as they can provide the effective configuration of MSSs for SPEs with high stiffness and high ionic stiffness with significant savings in computational cost.

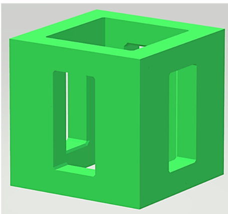
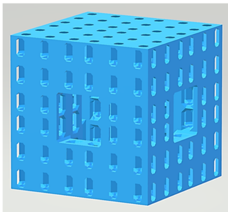
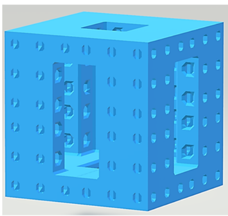
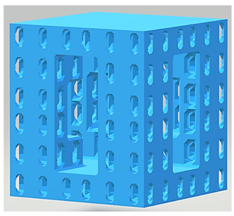
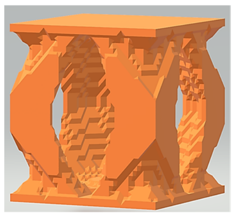
(a) Opt_Solid_L	(b) MSS_1	(c) MSS_2	(d) MSS_3	(e) Opt_Solid_H
				
Macro (d_f = 0.35), Micro (d_f = 1.0)	Macro (d_f = 0.7), Micro (d_f = 0.5)	Macro (d_f = 0.5), Micro (d_f = 0.7)	Macro (d_f = 0.59), Micro (d_f = 0.59)	Macro (d_f = 0.35), Micro (d_f = 1.0)

Figure. 7 MSSs of five different structures with the same overall density fraction ($\boldsymbol{d_{f,MSS} = 0.35}$) and dimensions of MSSs (36×36×36)

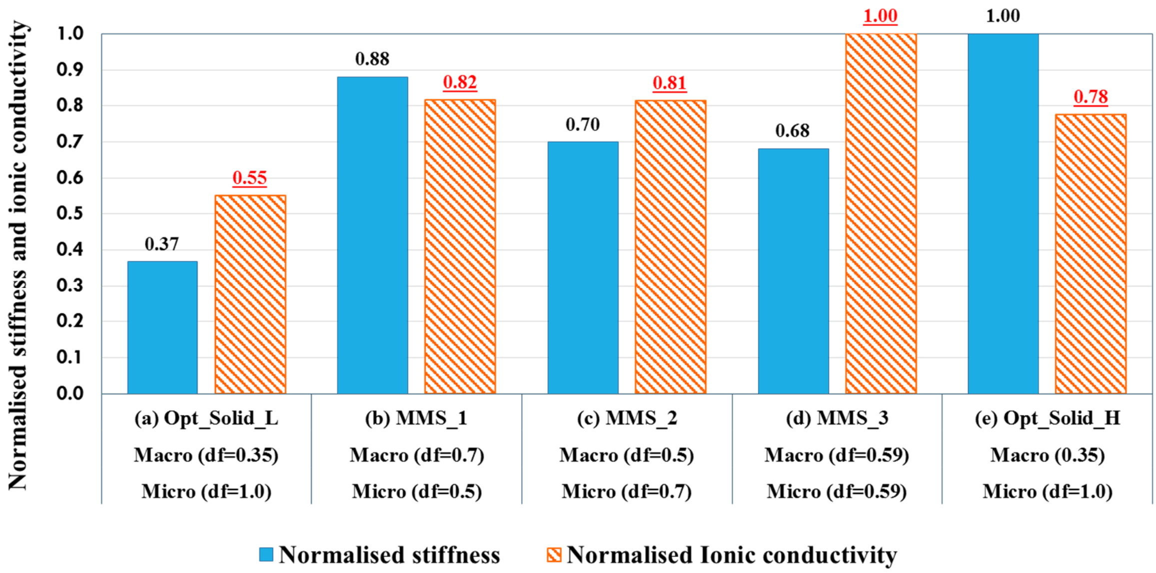


Figure. 8 Comparison of multifunctionality for five different multi-scale structures with uniform micro-scale structures (dimension 36×36×36)

5 Conclusions and future works

This study presents a novel design strategy to achieve optimised multi-scale structures (MSSs) for multifunctional polymer matrix with high structural stiffness and high ionic conductivity. We demonstrated the efficiency of our strategy by designing, optimising and evaluating two-scale structures composed of macro-and micro-scales. A database of optimised micro-scale structures and simple placement criterion of the micro-scale structure were applied. Particularly, we built the finite element model-based database composed of the optimised topologies of microstructures rather than averaged material properties.

To explore and evaluate the multifunctionality of MSSs, five different structures were constructed under uniaxial loading with the same density fraction (d_f); the stiffness and ionic conductivity of MSSs showed relatively high value compared to the maximum stiffness and ionic conductivity of the optimised solid and void structure. Hence, these results demonstrated that MSSs are very promising as they can provide the effective configuration of MSSs for SPEs with high stiffness and high ionic stiffness with significant savings in computational cost.

A future study will explore the optimised MSSs with a higher mesh resolution to consider a more accurate stress and strain distribution. The experimental validation of the proposed optimisation strategy and extended study for other multifunctionality also can be added in the future study.

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