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Safe energy-storage mechanical metamaterials via architecture design

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Abstract. Mechanical and functional properties of metamaterials could be simultaneously manipulated via their architectures. This study proposes multifunctional metamaterials possessing both load-bearing capacity and energy storage capability, comprising multi-phase lattice metamaterial and cylindrical battery cells. Defect phase are incorporated into the metamaterials, which are then printed with stainless steel powder. The printed metamaterials are assembled with battery cells and compressed. Experimental results revealed that the voids in the lattice metamaterials, could guide deformation mode away from the internal battery cell that postponed the emergence of battery short-circuit. Effects of void phase pattern and content are discussed by simulation. We found that the multifunctional system could absorb greater energy after defect phase incorporation, as designed with proper void phase pattern and content. Also, these findings are further validated for the system with six battery cells. This study demonstrated how to design an energy-storage metamaterials with enhanced mechanical properties and battery safety simultaneously. Also, defect engineering was helpful for battery protection and energy absorption of the multifunctional system.

Keywords: Mechanical metamaterials / digital design / battery safety / multifunctionality / defect engineering

1 Introduction

Mechanical metamaterials are those with ordered microstructures possessing unusual mechanical and functional properties. Many excellent works had been focused on how to achieve their unusual properties by tailoring architectures or using their uniques cellular characteristics, with the assistance of additive manufacturing technology, McMeeking et al. found that stiff but well distributed networks of plates could reach the Hashin-Shtrikman upper bounds, by evaluating the manner strain energy distributed [1]. Wegener et al. designed an elastic chiral mechanical metamaterials that could twist per axial strain as large as $2^0/\%$, which demonstrated artificial materials could be rationally designed to obtain an unexpected behavior [2]. Pham et al. designed a damage-tolerant metamaterials inspired by the hardening principles of metallurgy [3]. Valdevit et al. developed tensegrity metamaterials achieving delocalized deformation via the discontinuity of their compression members, which promoted the design of superior engineering system, from reusable impact protection systems to adaptive load-bearing structures [4]. By using the nature of their porous architecture, Lu et al. proved that mechanical metamaterials exhibited excellent heat transfer property and could be used as heat exchanger [5]. Recently, a dual-phase lattice metamaterial was proposed and developed, whose designing space for strength and energy absorption capability expanded significantly by manipulating the patterning of each phase [6,7]. This study shed light on the further digital design of multifunctional mechanical metamaterials by incorporating function as the separate phase.

Li-ion batteries (LIBs) became more and more prevailing power sources in electric vehicles, and the safety issues of LIBs had been widely concerned. Numerous researches had been taken on the mechanical abusive of LIBs. Wang et al. [8] built a detailed mechanical model describing the mechanical deformation and predicting the short-circuit onset of commercially available 18650 cylindrical battery. Besides, Liu et al. [9] established an internal short circuits model based on the battery pierce experiment, which shown a good prediction on battery safety. Moreover, machine learning was also used for predicting the battery risk. Jia et al. [10] developed data-driven

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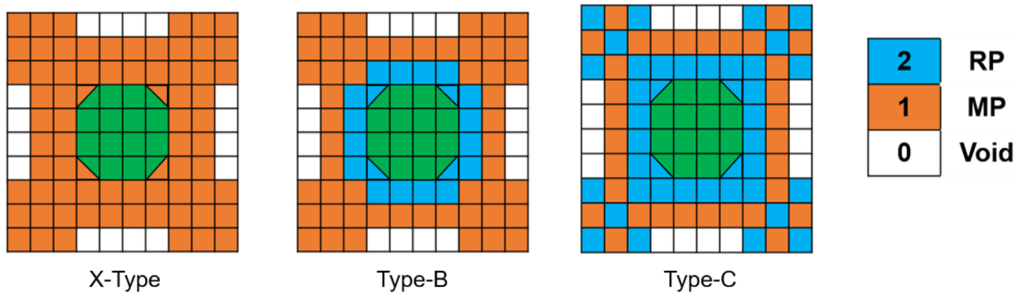

Fig. 1. The representative volume element (RVE) of the multifunctional structural battery system by digital design of constituting phase patterns of mechanical metamaterials: (a) Initial X-Type inspired from literature [14]. (b, c) Types-B and C with dual-phase lattices. Note that matrix phase (MP) are termed as phase 1, reinforcement phase (RP) as phase 2, and defect/void phase as phase 0.

models that can accurately predict the safety of LIBs under mechanical stress. However, how to improve battery safety at a system level was still demanded and urgent to be solved. Siegmund et al. [11] proposed a multifunctional and damage-tolerant battery system to enhance battery safety, whereby individual cylindrical battery units and sacrificial tubes were combined into a packing structure. Additionally, Shuai et al. [12] designed a new thin-walled honeycomb structure for LIBs packaging with optimized geometrical parameters for increased battery protection.

The objective of this study was to create a multifunctional digital metamaterial by simply incorporating lithium-ion battery cells as the energy phase while lattice metamaterials as the load-carrying phase, and thus possessed both energy storage and load-bearing capacity. Meanwhile, voids were observed in mantis shrimp and had been demonstrated to enhance the impact resistance of 3D printed bio-inspired composites [13]. Accordingly, in this study, the termed defect engineering was introduced into metamaterials design. How to protect the functional battery phase by microstructure design of the surrounding metamaterials we further examined based on our previous study [14]. Then, the designed lattice metamaterials were 3D printed and assembled with a single 18650 cylindrical battery. The deformation mode, load-displacement curve is monitored with the voltage variation. Finally, validated simulations are used to assess the performance for the multifunctional system with more battery cells.

2 Materials and method

2.1 Digital design

Multi-phase metamaterials are digitally designed with reinforcement phase (RP), matrix phase (MP) and defect phase, based on the previous topology optimization results, forming a representative volume element (RVE) of the multifunctional structural battery system after incorporating one cylindrical battery cell as function phase as shown in Figure 1. Body-centered cubic (BCC) combined with simple cubic (SC) lattice architecture is selected as the matrix phase (MP, termed as phase "1"), and face-centered cubic (FCC) combined with SC lattice architecture, as the reinforcement phase (RP, termed as phase "2"), as illustrated in Figure 2a in the following section. Additionally, defect/void phase is termed as phase 0, while the battery cell as function phase. The side length of each lattice unit is 5 mm with truss diameter of 0.7 mm, and the whole RVE consisted of 10 lattice units in total. Figure 1 shows three different types of phase patterns for mechanical metamaterials. X-Type is inspired from our previous study [14], while dual-phase lattices are incorporated aiming at enhancing the energy absorption capability. Their corresponding mechanical properties and battery protection capability will be explored and compared later.

2.2 Fabrication

The multi-phase metamaterials were fabricated by additive manufacturing using stainless steel powders. Selective laser melting (SLM) based additive manufacturing was adopted for the fabrication of metamaterials on an EOS M280 printer using stainless steel powder. The advantages of SLM included the production of flexibly customized, complex parts with a high resolution of 40 µm and remarkable mechanical properties. Before the heating process, a layer of AISI 316 L austenitic stainless-steel powder was spread on the surface of a building platen. A galvanometer was utilized to direct a laser beam across this surface to melt powder where necessary, fusing it with the layer below. Then the platen was lowered followed by the same fusing process, repeated until finishing. The fabricated samples were shown in Figure 2. Then, the multifunctional structural battery system was formed after inserting the battery cells undergoing a single discharging cycle to zero.

2.3 Mechanical testing

The digital metamaterial assembled with battery cells were compressed using in-situ voltage measurements via a voltage sensor to evaluate the protective capability of the system, and the compressive behavior of those with optimized dual-phase pattern was compared with that of the initially designed lattice pattern. All the specimens were compressed

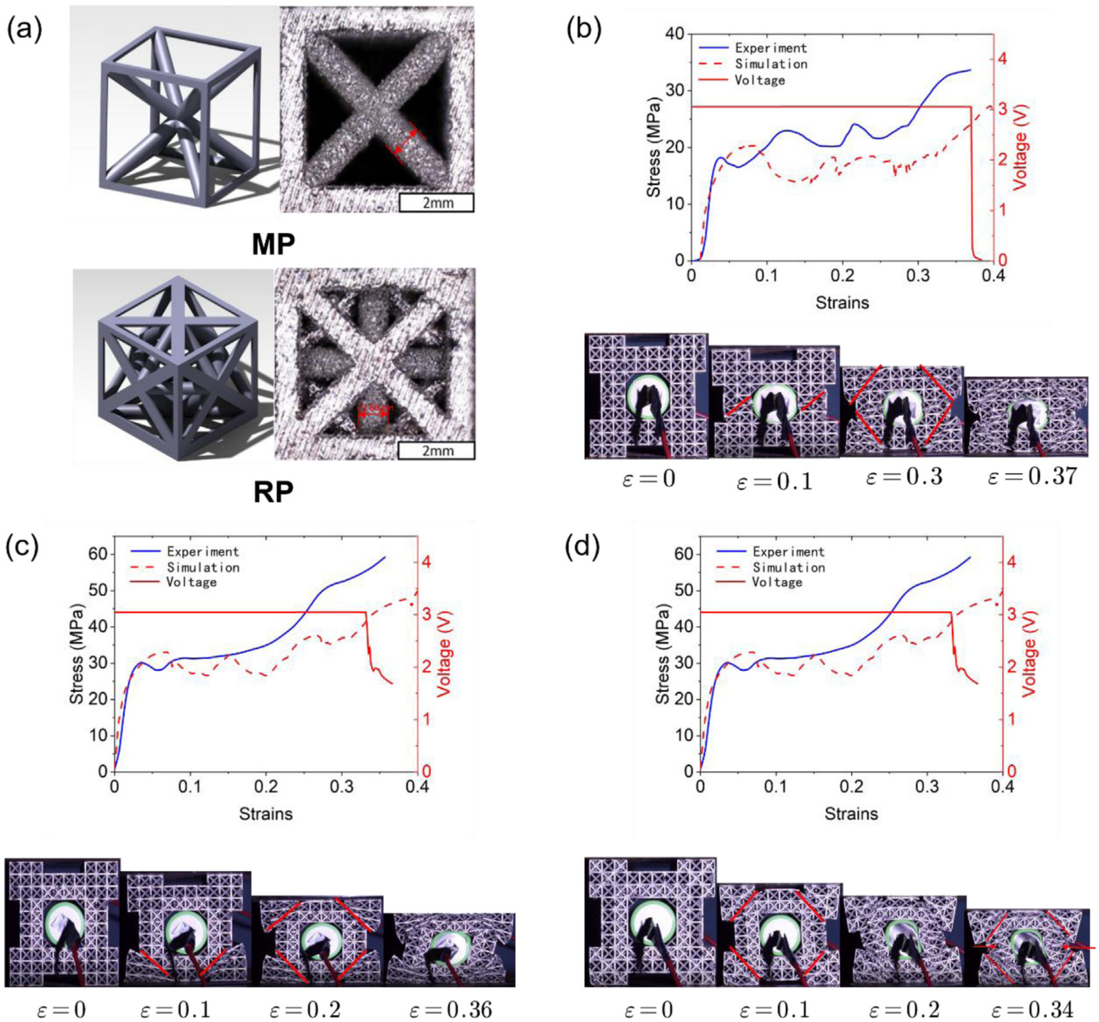

Fig. 2. Compression testing for the assembled structural battery system fabricated by SLM. (a) Mesoscopic truss morphology. (b, c, d) The voltage curve, engineering stress-strain curves, and deformation modes of the multfunctional system with different types of patterns.

on a universal electromechanical testing machine (MTS Exceed E64, MTS Systems China, Shenzhen) at a constant cross-head strain rate of ~10^{-3}/s. At least three tests were carried out for each group of specimens to ensure repeatability. The morphology and failure modes after the compression tests for all the samples were observed in a KEYENCE VHX-6000 optical microscope (Keyence, Osaka, Japan). Furthermore, videos were also recorded during the compression testing for further analysis.

2.4 Simulation

Finite element analysis (FEA) is performed to further investigate the stress distribution within the system during compression, using an explicit dynamics FEA approach (Radioss, Altair, USA). For the whole model, lattices meshed with beam elements possessing the experimentally measured diameter, while the battery cell with solid elements. Then, the units are compressed between two stiff plates both meshed with solid elements. A mesh convergence analysis is performed to select the appropriate element size, whereby an element size of 0.5 mm is selected for the beam and solid elements to ensure accurate results with a high calculation efficiency. The properties of metamaterials are set to be ideally elastoplastic in the simulation model. Moreover, the battery is set as a foam model and validated by comparison with experimental results from our previous study of a single 18650 battery cell during radial compression [8]. In this model, two types of contacts were employed. The first is a line-to-line contact that simulated the contact among lattice trusses. The second is a line-to-surface contact between the lattice trusses and the compression plates/LIB cells.

To validate this compression model, the simulated stress–strain curves and deformation modes are compared with experimental results for all three types of structures as

Table 1. Summary of mechanical properties of the multifunctional metamaterial system with different phase patterns.

Pattern	Strength (MPa)	Stiffness (MPa)	Battery short-circuit strain	Energy absorption (J)
X-type	18.1	550.0	0.37	750.7
Type-B	22.1	1128.3	0.36	941.4
Type-C	30.2	1750.5	0.34	1246.7

shown in Figure 2. The simulated stress-strain curves are consistent with the experimental curves in the elastic segment while there was a certain difference in the subsequent stages, as the nodal volume effects could not be neglected for lattice materials with a greater relative density during compression, and the beam element cannot accurately simulate the numerical value. Furthermore, the distribution of shear bands in the simulation results was almost the same as that observed experimentally. The results indicated that FEM could predict well the deformation mode of the multifunctional system.

3 Results and discussion

3.1 Compressive response

The compressive (engineering) stress-strain curves with their corresponding deformation history are shown in Figures 2b and 2c. For those with initial X-type pattern, a shear band appeared in the metamaterials around the battery after the first stress peak ($\varepsilon = 0$–0.1), deducing the battery cell to be squeezed by the surrounding materials directly. Then, four shear bands occurred at the four corners of RVE ($\varepsilon = 0.1$–0.3), which was affected by voids where local structural stiffness decreased, accompanying with two stress peaks. Note that the battery cell kept working normally, attributed by its stronger mechanical properties than lattice materials, even though being compressed by the surrounding lattice metamaterials. Battery short-circuit occurred at strain of 0.37 after the whole system were densified.

As for those with Type-B pattern that RP closely wrapped the battery cell, the deformation process was divided into two stages. At first, the matrix phase deformed and shear bands gradually formed at the junction between MP and RP, while RP and battery are rarely deformed ($\varepsilon = 0$–0.2). Then, as further compressed, the battery cell and RP began to deform deducing stress increase until densification as shown in Figure 2c. Battery short-circuit occurred at strain of ~0.36 when the surrounding RP fully deformed and could not protect the inside battery cell.

To further improve the battery protection capability, energy absorption before short-circuit should be increased. Based on the previous study [6], Type-C patterned dual-phase metamaterials are examined as shown in Figure 2d. The deformation mode was rather similar with that of Type-B patterned materials; however, transverse compression on battery occurred which would prolong the battery short-circuit mainly deduced by vertical compression previously. The peak stress and energy absorption before battery short-circuit are analyzed and summarized in Table 1. Note that the energy absorption capablity for the multifunctional system with Type-C patterned metamaterials was 1246.7 J, 66% greater than that with X-type, and 33% greater than that with Type-B patterned metamaterials.

3.2 The role of defects on deformation

Comparing with the previous study, voids are found to played an important role in guiding deformation of the whole system, and effects of void shape and content are discussed.

3.2.1 Effects of void phase pattern

The pattern of void phase could control the deformation pattern of the system, and thus the desired deformation mode could be obtained by designing void-phase patterning. Here, two different void shapes designed as trapezoids and rectangles with the same void ratio are simulated, and results exhibited different deformation modes. With the trapezoid-shaped voids, as the red line indicated, the main deformation was transverse compression, because the lateral stiffness with the existing of voids was the lowest and thus prone to deform. From the simulation, we found that the battery cell started to deform at the strain of 0.09, which was quite early comparing with other patterns.

Otherwise, with the rectangle shaped voids, metamaterials deformed similar to that observed in the previous experiments, and the main deformation occurred at the corners resulting in four shear bands. The battery cell started to deform at the strain of 0.23, which enabled a longer deformation stage and would contribute to energy absorption capability. Accordingly, a proper designed shape of defects could regulate the deformation mode during compression and prolong battery failure or short-circuit.

3.2.2 Effects of void content

Void content could also affect the deformation pattern and battery protection. Rectangle shaped voids was chosen for discussion, and the number of void phase units k varying from 0, 2, 4, and 6 are analyzed and discussed (Fig. 3b). Note that the local stiffness varied with void number, and thus the deformation modes are different. The red line indicated the simulated shear band position as the battery being compressed.

With $k = 0$, the battery started to bear load and being squeezed at strain of 0.08, and localized shear band (Fig. 3b - I) indicated that the battery would be compressed directly. For $k = 2$, shear band occurred at the position as indicated, and the battery would start to bear load at strain of 0.1 after the surrounding metamaterials collapsed. As for $k = 4$ and 6, the system deformed similarly, and the shear

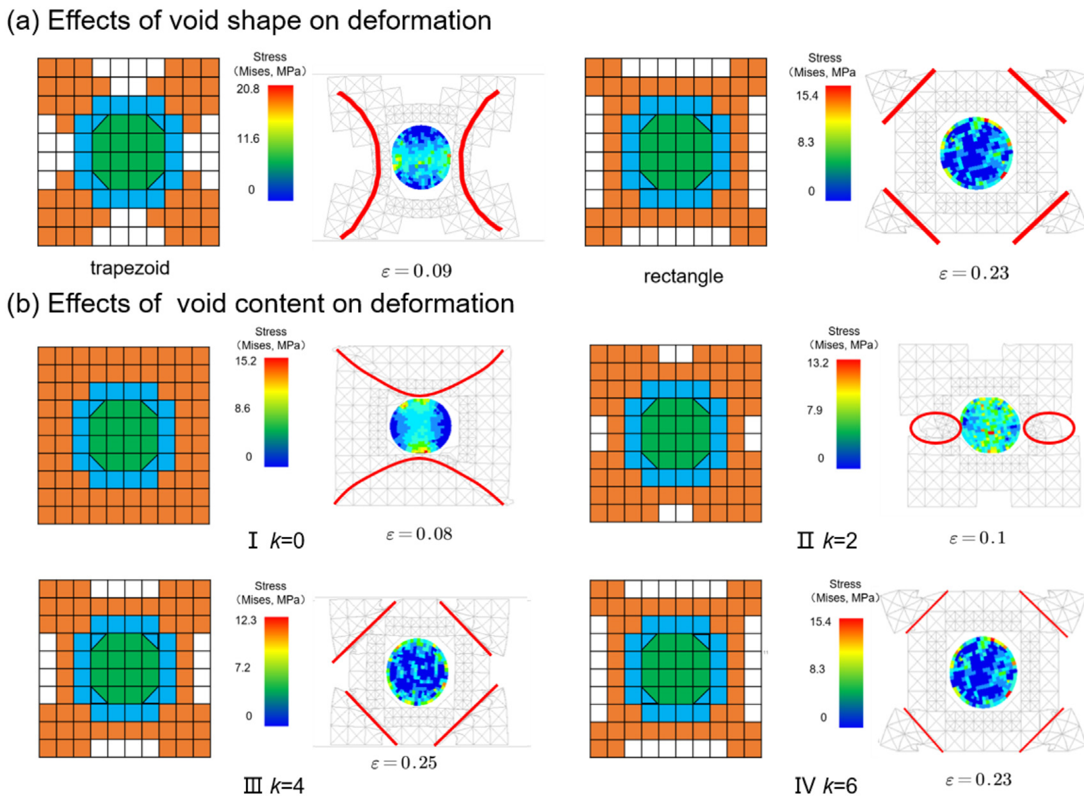

Fig. 3. The role of voids/defects on deformation. (a) Effects of void shape on deformation; (b) Effects of void content on deformation, and (I–IV) corresponds to the numbers of void-phase unit k varying from 0, 2, 4, and 6.

Table 2. Effects of void shape and number on battery protection.

Void phase pattern	Number of void phase units, k	Battery load-carrying strain	Energy absorption (J)
Triangle	6	0.09	87.2
Rectangle	0	0.08	279.5
	2	0.1	301.6
	4	0.25	474.5
	6	0.23	295.1

band for those with $k = 6$ moved outward more clearly. However, note that the energy absorption of the whole system, as summarized in Table 2, increased with k, while decreased again as the void unit number $k = 6$. Accordingly, it's indicated that the defects could guide the deformation mode and only increase the energy absorption with proper void content.

3.3 With multiple battery cells

With six battery cells, we further examine that whether the designed energy storage system with defects is superior to the uniform lattice-based system. Those with Type-B and Type C patterned metamaterials are designed and compared with those without any voids as shown in Figure 4 and Table 3. Similarly, the strain as battery cell started to carry load is employed as the designing criteria for comparison. Results show that voids in the multifunctional system with six battery cells, can also guide the deformation mode and shear bands distribution; meanwhile, the battery load-carrying strain is postponed by 125%. Also, the energy absorption increases by 54.5% for Type-B patterned system while 74.8% for Type-C patterned one, although the existence of voids will reduce stiffness and strength. Comparing those with Type-B patterned metamaterials, the dual-phase metamaterials incorporation into the matrix phase (Fig. 4c), further increases the energy absorption by ~32% without affecting the deformation mode. Note that the stress level of the middle battery cell will be relatively higher (Fig. 4c) because of the limited deformation space of this RVE comparing with the other ones in the system with free boundary condition. Accordingly, trusses will buckle easily in this RVE deducing the battery being compressed first. Actually, the stress level will be more balanced for a practical battery back with multiple battery cells.

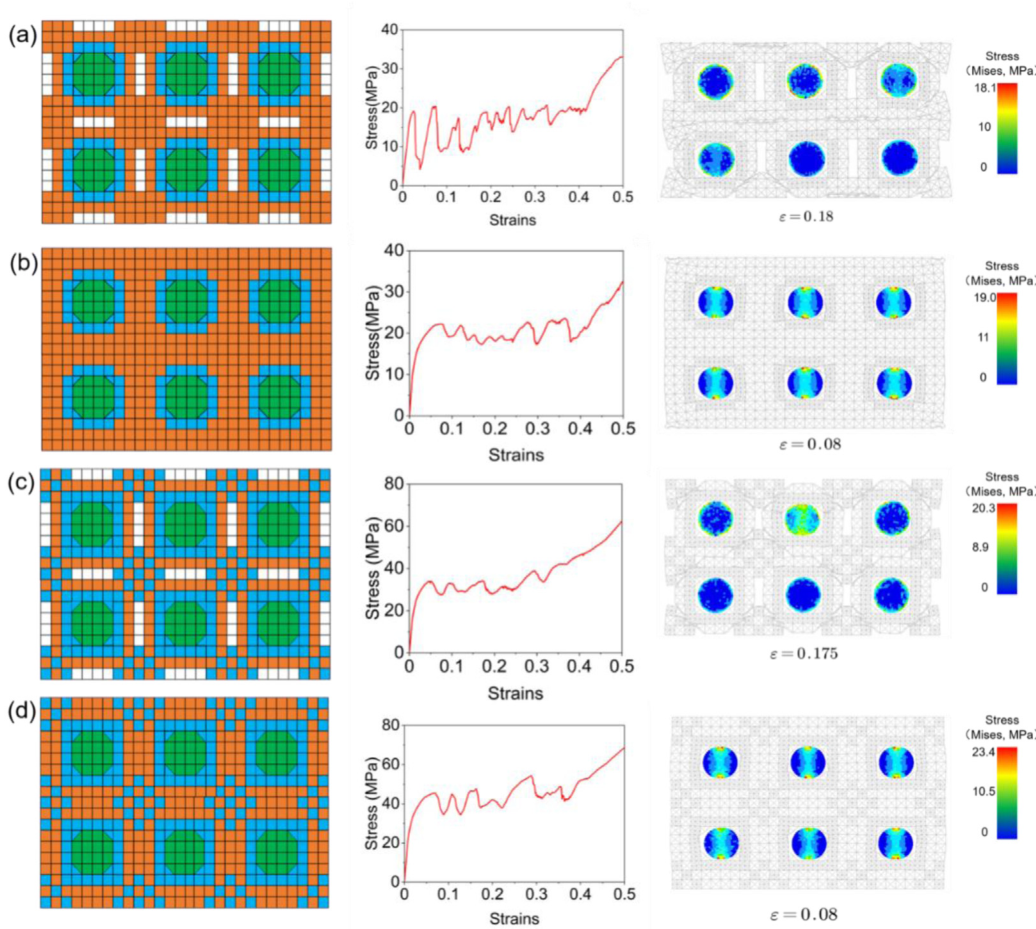

Fig. 4. Simulation of the multifunctional energy storage system with or without voids under compression. (a, b) Systems with Type-B RVE comparing those without voids. (c, d) Systems with Type-C RVE comparing with those without voids.

Table 3. Summary of mechanical properties of the multifunctional systems with multiple battery cells.

Pattern	Voids	Strength (MPa)	Stiffness (MPa)	Battery load-carrying strain	Energy absorption (J)
Type-B	Yes	20.3	856.3	0.18	1927.9
	No	25.6	840	0.08	1248
Type-C	Yes	35.7	1168	0.175	2558.4
	No	45.2	1590.9	0.08	1463.8

4 Conclusion

Functionality could be realized for mechanical metamaterials via digital design of constituting phases. This study proposes multifunctional metamaterials possessing both load-bearing capacity and energy storage capability, comprising multi-phase lattice metamaterial and cylindrical battery cells. Bioinspired defect phase is incorporated into metamaterials, which are then printed with stainless steel powder before assembling with battery cells. The assembled structural battery system is lighter than that without voids in our previous study, and compressed. Experimental results reveal that the voids in the lattice metamaterials could guide deformation mode, postpone the internal battery cell short circuit. Effects of void phase pattern and content are also discussed by simulation. We found that the multifunctional system could absorb greater energy after defect phase incorporation, as designed with proper void phase pattern and content. Also, these findings are further validated on the system with multiple battery cells. This study demonstrated how to design an energy-storage metamaterials with enhanced mechanical properties and battery safety simultaneously via architecture manipulating. Also, defect engineering is helpful for both battery protection and energy absorption of the multifunctional system. Data-driven based machine learning may be used for further optimization of mechancial metamaterials to achieve functionality, such as the next generation of lightweight and safe energy storage system.

Declaration of interests

The authors declare no competing interests.

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