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Design of hierarchical lattice structures attainable by additive manufacturing techniques

L Musenich, A Stagni and F Libonati

University of Genoa, Department of Mechanical, Energy, Management and Transportation Engineering, Via all'Opera Pia 15/A, 16145, Genova, Italy

flavia.libonati@unige.it

Abstract. Readiness of new materials that are simultaneously lightweight, damageresistant, multifunctional, and sustainable is a primary need for many technology sectors. Thanks to additive manufacturing, lattice materials appear to be ideal candidates to meet this challenge. By designing their unit cells and structural organization, multiscale materials with unique combinations of properties can be obtained. Nevertheless, many gaps remain to be filled for their effective and efficient design. Nature, exploiting hierarchical architectures on a material scale, actually amplifies the properties of biological materials and combines them in ways we cannot achieve yet in synthetic materials. In materials design, we are still far from such a level of perfection. To narrow this gap and expand the current knowledge on the effects of hierarchy on the mechanical behaviour of materials, we numerically studied the mechanical response of 3D hierarchical lattice specimens under a four-point bending loading scenario. For this, we selected two types of unit cells with different structural behaviour and combined them together into different specimen topologies. The results show that, through hierarchy, it is possible to tailor lattice material performances, achieving benefits in terms of both specific mechanical properties and multifunctionality. The evidence found opens new horizons for applications such as heat exchangers, mechanical filters, scaffolds, energy storage, and packaging.

1. Introduction

Sustainable development requires the search for new technological solutions that can preserve and improve the quality of life by promoting a circular economy aimed at protecting natural resources and minimizing the ecological footprint. In the field of materials design, this translates into the research of methods and tools to fabricate high-performance materials (i.e., lightweight, damage-tolerant, and multifunctional) by using a limited number of resources, thus reducing the environmental impact and increasing the recycling likelihood. Nature is a master in this field. Indeed, natural composite materials such as bone, mother-of-pearl, or wood teach us that such performances can be achieved through complex bottom-up multiscale design and building logic [1-4]. Although the recent advances in manufacturing it is not possible to achieve such details at the material scale yet. Lattice materials, thanks to the development of additive manufacturing techniques, are offering a very promising opportunity to narrow this technological gap that exists between Nature and engineering [5-12].

Lattice materials are made of a combination of elementary building blocks (known as unit cells, u.c.s) that are repeated in space. This peculiarity makes lattice materials to behave as structures at the u.c.

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scale (meso scale) and as materials at the macro scale [13–15]. Thanks to their structure, lattice materials can be architected, including structural heterogeneities and multiscale substructures, to achieve combinations of properties not found in conventional engineering materials. The multiple design degrees of freedom that lattice materials offer make the characterization of the property-process-structure-performance relationship (PSPP relationship) very complicated. To date, there are many challenges to overcome for their optimal implementation in engineering applications [16–18]. Indeed, from literature, it is known that the apparent mechanical behavior of lattice materials at the macro scale can be described as a function of: (i) the base material properties, (ii) the u.c. connectivity, and (iii) the relative density [14]. Depending on u.c. topology, lattice u.c. have also been classified into two macro-families characterized by distinct mechanical behaviors: bending- and stretching-dominated, respectively [14,19]. However, it is not entirely clear how the combination of different lattice u.c. at different length scales can change the material performance.

Optimizing the structural organization of fractal-like hierarchical 2D lattice materials, elastic properties can be adjusted within a wide range and some of the structure may benefit from the hierarchical architecture [20–22]. In addition, not only the elastic properties, but also crack propagation can be controlled and enhanced through the implementations of a multiscale design [23]. Similar results were also found for three-dimensional ones. Specifically, in terms of stiffness, it has been observed that bending-dominated lattice u.c.s benefit from a hierarchical architecture to a greater extent than stretching-dominated ones [24]. Yet, the presence of more hierarchical levels produces higher stress concentrations that reduce the overall strength of the material. Also, beyond two levels of hierarchy, it is hard to obtain appreciable gains on the performance of lattice materials [25].

Combining bending-dominated and stretching-dominated u.c.s in hybrid-type hierarchical lattice structures unique properties can also be obtained. Such structures have been conventionally identified with names consisting of two parts: "x-y" [26–28], where "x" denotes the type of structure on the largest reference length scale and "y" that on the smallest length scale. We follow this convention in our work. Stiffness and elastic buckling resistance of multiscale bending-bending lattices progressively improve with hierarchy, while for stretching-stretching lattices the increase in buckling resistance is accompanied by a reduction in stiffness. Bending-stretching lattices are at the same time less stiff and less strong [26]. In determining the mechanical response of lattice materials, the slenderness ratios of u.c. struts at different hierarchical levels play a key role [29].

Literature findings presented above are mainly derived from numerical analyses of the deformation of lattice materials under compressive loading condition and do not provide comprehensive design guidelines. Therefore, to extend the current knowledge on the PSPP relationship of multiscale lattice materials, in this work we analyze the mechanical performance of 3D lattice structures at two levels of hierarchy, subjected to bending. To evaluate the benefits obtainable from exploiting substructures with different behaviors, we chose two different types of "strut-based" elementary u.c., one bending-dominated and one stretching-dominated. Then we combined them into six different structural topologies. Through finite element (FE) simulations, we analyzed the influence of the u.c. struts slenderness ratio on their mechanical behavior. With a view to extending this study, the geometries of the lattice models and their material properties were assigned based on the Fused Filament Fabrication (FFF) 3D printer constraints, for the purpose of future experimental validation.

2. Materials and Methods

2.1. Hierarchical lattice structure modelling

As a case study, we considered a specimen subjected to 4-point bending (4PB) loading. The study of a bending loading scenario allowed us to work on a design space with a simple geometry but, at the same time, characterized by gradient stress states, which opens up the design of lattice structural topologies in view of optimal material utilization. In addition, since in the 4PB configuration a larger portion of the

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specimen is affected by a constant bending moment, discontinuities, peculiar to lattice structures, are mediated over a larger volume.

We defined our design volume as a 4-by-4 u.c. square section specimen (H= 48 mm) and 32 u.c. along the longitudinal dimension (L = 192 mm). The pin distances were set to 144 mm and 48 mm for the supporting and for the pushing pins respectively.

Then, we voxelized the design space into cubic sub volumes with 12 mm edges with the idea of substituting each voxel with a specific type of lattice unit cell. We defined the dimensions of the voxels, and thus the u.c., on the basis of printing tests carried out with a Prusa i3 MK3S Original kit 3D printer having a 0.4 mm nozzle and using a commercial bio-based filament (polylactic acid, PLA).

To populate the design space, we chose two types of u.c. (i.e., non-hierarchical u.c., NH-u.c.) that are characterized by different mechanical behaviors, good geometric compatibility, and that are easy to be 3D printed: the bending dominated simple cubic cell (SC) and the stretching dominated face-centered cubic cell (FCC). A qualitative representation of their different behavior and a general representation of the followed workflow is visible in figure 1.



Figure 1. Representation of the study rationale. We first selected the SC and FCC lattice u.c.s for their different mechanical behaviour and good geometric compatibility. Then we populate a beam specimen –voxel by voxel–with the chosen u.c.s. The specimen has square cross section and nominal dimensions L = 192 mm and H = 48 mm and is subjected to a 4PB load. In the figure F represents the reaction force, u the imposed displacement and δ the maximum specimen deflection.

Combining the selected unit cells at different levels, we were able to introduce structural hierarchy in the specimen. To obtain the hierarchical u.c. (H-u.c.), we exploited a nested logic: we emptied the material present in the above-mentioned unit cell struts and substituted it with arrays composed of five SC or FCC unit cells. A representation of the hierarchical unit cell modeling logic adopted is shown in figure 2(a), while figure 2(b) depicts the four types of H-u.c. that we obtained by combining SC and FCC cells on two different length scales. Following the convention used in literature [26–28], the names of the H-u.c. were defined through acronyms consisting of two parts: "x-y", where "x" describes the level 1, and "y" describes the level 2. H-u.c. also can be classified into two families: self-similar H-u.c., i.e., those obtained by combining different types of NH-u.c. (SC-FCC models), and hybrid H-u.c., i.e., those obtained by combining different types of NH-u.c. (SC-FCC and FCC-SC models). To comply with the constraints imposed by the 3D printer mentioned above the edge length of the NH-u.c. was set equal to 12 mm while for the H-u.c. edge length was set at 3 mm (figure 2(a)).

With the defined lattice u.c. we created six different architected lattice specimens, two nonhierarchical (NH-specimens) and four hierarchical (H-specimens). The six models were obtained by substituting in the entire design space the SC, FCC, SC-SC, SC-FCC, FCC-SC, FCC-FCC u.c., respectively. The representation of the different specimens is showed in figure 3.



Figure 2. Hierarchical design of lattice unit cells: (a) representation of the modelled structural levels; (b) schematization of the four different hierarchical (or level 2) u.c. used in our work. The edge length dimensions used for this study are equal to 12 mm and to 3 mm for the NH-u.c. and the H-u.c. respectively.

The names of the four lattice specimens' configurations echo those of the unit cells used to populate the design space and are indicative of the behavior of the different structures. For example, the SC-FCC specimen has the SC structure at the macro level and the FCC structure at the meso level. Thus, it is a specimen characterized by hybrid bending-stretching behavior.

2.2. Numerical simulations

To investigate the mechanical behavior of the architected lattice specimens, we set up numerical simulations in ANSYS Mechanical APDL. This software allowed us to efficiently formulate customized calculation routines (i.e., macros) capable of correctly defining the architected u.c. and combine them together to create the specimen geometries in an automated manner. Parametric lattice specimen models were defined using 3D 2 node beam elements with linear shape function (beam 188 with KEYOPT(3)=0 in the Ansys MAPDL element library). An iterative cycle was set up to automatically compute the solution of the different designs. The use of beam elements, despite allowing only a simplified representation of the real phenomena to be studied, made it possible to evaluate about 50 different geometric configurations in a reasonable time frame and with limited computational costs. The exploitation of geometrical symmetry, material properties, and boundary conditions, present in all the designed lattice models, made it possible to further speed up the analyses.

All the simulations were performed in displacement control, assigning a negative deflection u = 0.3 mm to the nodes of the finite element models located under the bending pins. A convergence analysis was done to define the maximum size of the FE mesh. Specifically, in the NH-specimens each strut was discretized into ten beam elements, while for the H-specimens each strut of the smallest u.c. was represented by two FEs. A homogeneous and isotropic linear elastic material model was used. Material properties were derived from an experimental campaign of a commercial PLA filament.



Figure 3. Front view representation of the modelled non-hierarchical (top) and hierarchical (bottom) lattice specimens. The specimens are symmetrical with respect to their midplane, so for each model, we depicted only one half.

2.3. Performance metrics

We analyzed the performance of the lattice specimens designed in terms of stiffness through four different metrics. To characterize our specimens as structures, we used the slenderness ratio (s.r.) of the u.c. lattice struts and the bending stiffness (K_b) of the specimen, defined respectively as:

$$s.r.=d/l$$
 (1)

$$K_{\rm b} = F/\delta$$
 (2)

where d and l are the strut diameter and strut length of the smallest u.c. (see figure 4), respectively; F is the force exerted by the bending pins, δ is the maximum deflection experienced by the specimen (see figure 1).

Once the u.c. edge length has been fixed, we set the s.r. range from 0.15 to 0.45, then the strut diameters were calculated accordingly. The same s.r. were used for both the H-u.c. and the NH-u.c.. This strategy for defining the s.r. is consistent with previous studies [29].

To characterize our specimens as materials we employ the relative density (ρ_{rel}) and the relative elastic modulus (E_{rel}) of the lattice material, defined respectively as:

$$\rho_{\rm rel} = \rho^* / \rho_{\rm bulk} \tag{3}$$

$$E_{rel} = E^* / E_{bulk}$$
(4)

where ρ^* and E^* are the apparent density and the apparent modulus of the lattice structure, and ρ_{bulk} and E_{bulk} are the density and the Young modulus of the base material, respectively.



Figure 4. Geometric control parameters of the lattice unit cell: l represents the length of the strut and d the strut diameter.

3. Results and discussion

3.1. Structural hierarchy effect

We first analyzed the effect of structural hierarchy on the stiffness of lattice specimens. figure 5(a) shows the stiffness of the lattice specimens as a function of the slenderness ratio of the u.c. struts, while figure 5(b) shows the same plot but with the stiffness normalized to the weight W of the lattice specimens.



Figure 5. Finite element analysis results of lattice specimen models. (a) Trend of the lattice specimen stiffness as a function of the slenderness ratio of the lattice unit cell struts. (b) Trend of lattice specimen stiffness normalized to their weight as a function of the slenderness ratio of the lattice unit cell struts.

As expected, based on literature results [14], the NH-specimens show significantly different behavior: both show an increase in stiffness as the slenderness ratio of the u.c. struts (and thus their diameter) increases (see figure 5(a)), but the stretching-dominated FCC specimens are much more efficient. Indeed, at the same s.r., they show consistently higher performance than non-hierarchical bending-dominated lattice specimens. Moreover, regardless of their weight, they keep approximately constant structural performance within the considered s.r. range (see figure 5(b)).

Looking at the results for H-specimens, on the other hand, it can be seen that-in terms of stiffness (see figure 5(a))-the introduction of stretching-dominated FCC substructures does not appreciably

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change the mechanical behavior of lattice specimens, while the introduction of bending-dominated SC substructures is not advantageous, as it leads to worse performance than NH-specimens. Looking at the weight-normalized performances (see figure 5(b)), there is a significant change in slope between hierarchical and non-hierarchical structures, regardless of the type of substructure present at level 2. Specifically, reasoning from a lightening viewpoint, we can say that hierarchy is only beneficial when introduced in bending-dominated NH-specimens since, as the amount of material used decreases, the loss of stiffness they exhibit compared to non-hierarchical models is less. For non-hierarchical stretching-dominated specimens, structural hierarchy is advantageous only if, assigned a specific value of s.r., stretching-dominated lattices are introduced at level 2, as they lead to better performance than the corresponding NH-specimens.

3.2. Scaling laws

Then we investigated the behavior of lattice specimens through homogenized properties and thus as equivalent materials. It is known, from the literature [14], that the scaling law of the relative elastic modulus of lattice materials with their relative density is of the type:

$$E_{rel} \propto \rho_{rel}^n \tag{5}$$

where the exponent n takes value 2 for bending-dominated structures and 1 for stretching-dominated structures [14]. We then used these results as a benchmark for the analysis of the models we built. Figure 6 shows the interpolating curves representing the scaling laws of the relative elastic modulus as the relative densities of the lattice specimens we modeled. Table 1 shows the numerical values of the scaling law exponents of the studied lattice materials and the corresponding theoretical values for the bending-and stretching-dominated cases.



Figure 6. Scaling laws of relative elastic modulus for numerically simulated lattice specimen models.

We can see from these results that the self-similar hierarchical lattice structures, i.e., bending-bending (SC-SC) or stretching-stretching (FCC-FCC) keep the same trends as the corresponding NH-structures (SC and FCC, respectively), allowing the application range of these materials to be extended more or less significantly. On the contrary, the hybrid hierarchical lattice structures, i.e., bending-stretching (SC-FCC) and stretching-bending (FCC-SC), exhibit different trends than the lattice structures from which they were derived. In general, it can be said that hybridization leads to structures that are prone to bending-dominated behaviour.

Scaling law exponent				
Model	n			
Bending dominated	2.00	Theoretical behavior		
Stretching dominated	1.00			
SC	1.60	Numerical results		
SC-SC	1.66			
SC-FCC	1.73			
FCC	1.10			
FCC-SC	1.30			
FCC-FCC	1.13			

Table 1. Scaling law exponents: theoretical values and numerical values, obtained from the FE-simulation performed in this study.

4. Conclusions

In our work we set up a parametric and automated numerical framework to systematically analyse NHand H- lattice specimens under 4PB loading scenario. In total we look at six different specimen topologies. Two NH-specimens, which we constructed by uniformly filling the design space with bending-dominated SC or stretching-dominated FCC lattice u.c.s, and four H-specimens, which we built by combining the same type of NH-u.c.s (SC-SC and FCC-FCC i.e., self-similar models) and the two different types of NH-u.c.s (SC-FCC and FCC-SC i.e., hybrid models). Changing their geometrical parameters, more than forty configurations were calculated. From the obtained results, the hierarchical self-similar lattice structures showed scaling laws of the relative elastic modulus with respect to the relative density very similar to those of the non-hierarchical lattice structures from which they were derived, whilst in terms of structural stiffness they showed significant changes in the mechanical efficiency of the specimens in bending. This means that self-similar structural hierarchy can be advantageously exploited to lighten structural parts and/or increase their specific mechanical performance (i.e., K_b, E_{rel}). Bending-stretching or stretching-bending structural hybridization, on the other hand, has led to materials with significantly different scaling laws than those of non-hierarchical lattice structures. Also, generalizing according to literature [24,26], is advantageous in terms of stiffness only if the structural hierarchy is designed by introducing stretching-dominated substructures within bending-dominated lattices. For both classes of the above-mentioned lattice specimens, the mechanical behaviour seems to be predominantly determined by the structural organization on the macro scale and thus by level 1 or non-hierarchical.

Looking beyond mechanical functions, the structural hierarchy opens the way for applications where lattice materials can perform multiple functions simultaneously. Specifically, one feature of lattice structures that undergoes significant changes with hierarchy is the surface-to-volume ratio. The latter greatly influences capabilities such as heat transfer, mechanical filtering, and shielding to electromagnetic waves. Therefore, extending the understanding of the PSPP relationship is of paramount importance not only in the field of mechanical design. This preliminary study lays the foundation for further analytical, experimental, and numerical investigations aimed at extending the characterization of hierarchical lattice materials subjected to bending loads from a multidisciplinary perspective, including the effect of local relative density gradients or material properties resulting from combinations of heterogeneous structures over multiple length scales.

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