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ARCHITECTURED AND ADDITIVELY MANUFACTURED DOUBLE-NEGATIVE INDEX METAMATERIALS

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Abstract. Developing a new generation of multifunctional metamaterials with unusual thermoelastic properties enables a wide range of industrial applications, particularly in the aerospace industry. However, obtaining metamaterials with target properties by the systematic design of their microstructure and architecture remains a major challenge to this day. Topology Optimization (TO) is a powerful tool that can be used to develop the so-called anepectic metamaterials that combine both negative Poisson's Ratio (NPR) and negative thermal expansion (NTE). Here, an overview of the existing contributions in the literature regarding such metamaterials is presented. A Finite Element (FE) model for an anepectic microstructure is presented here for the purpose of simulating *in silico* the experimental results obtained in previous works. It is noted that scarce contributions resort to TO to design such metamaterials and even fewer present experimental validation. The present work presents a state of the art of anepectic metamaterials and emphasizes thus the importance of the engineering-cycle completion, i.e., starting with the systematic and optimal design of metamaterials and ending up in prototype fabrication and its verification.

1 INTRODUCTION

Metamaterials are engineered materials that present unusual and attractive properties due to the spatial arrangement of their internal structure. Out of these properties, negative indexes, like negative Poisson's Ratio (NPR) and negative thermal expansion (NTE) stand out due to their wide range of applications, especially in the medical, aerospace and defense industries [1]. While materials exhibiting only one of these properties individually have been widely studied in the literature [2], contributions combining both negative indexes are scarce and especially presenting experimental validation [3]. In an effort to find feasible solutions for a real-life engineering problem it is important to complete an engineering cycle, i.e., one must start by identifying the problem, followed by the design, modeling, fabrication and testing prototypes.

One starts at a conceptual design stage of product development, but it is essential to follow then the next steps toward the use of metamaterials in real applications.

Metamaterials are engineered or architectured materials, as their properties can be derived from the architecture of a representative volume element, unit cell or microstructure, which is periodically repeated throughout the space. The design of these materials can be empirical, relying mostly on the experience and intuition of the designer. However, to fully explore the potential offered by these materials, systematic design methods, as Topology Optimization (TO), are quite promising. The inverse homogenization method in the frame of TO has been proposed. It finds the optimal material distribution within the unit cell domain such that the metamaterial has the desired properties [4]. The homogenization theory is valid only if the optimization problem verifies the following hypotheses: a) Infinite periodicity of the unit-cell, i.e., the microscale is infinitely small compared to the macroscale such that there is a scale separation; b) the unit-cell has periodic boundary conditions (BC's) and c) the macroscopic applied field, e.g., stress or strain, are uniform. However, in practical applications the composite material comprises a finite number of unit-cell repetitions. To simulate how the composite properties are affected by finite repetitions it is important to perform Finite Element Analysis (FEA).

In general, the metamaterial is auxetic when its micro-geometry configuration (e.g., re-entrant, chiral) forces the ribs to move outwards in the horizontal direction, when a vertical strain is applied. This deformation mechanism can be achieved with a single material present in the microstructure. However, to achieve the thermo-auxetic (anepectic) behavior, a common approach is to insert at least two different materials exhibiting distinct coefficients of thermal expansion (CTE) within an auxetic geometry. The placement of these materials is such that one material expands more than the other, causing the overall structure to shrink under temperature increase. Therefore, when designing anepectic materials, is common to consider multi-material solutions.

Most contributions in the literature follow the empirical design approach, i.e., the anepectic behavior is achieved on account of adapting the micro-geometry and materials placement in the frame of known auxetic microstructures [5-19]. As for the systematic design approach, although it has been widely used in the past three decades to design metamaterials exhibiting NPR or NTE individually [20,21], only three recent contributions exist addressing the anepectic behavior as far as the authors know [22-24]. In Figure 1 a summary of anepectic meshes found in the literature is presented. Notice that almost half of these studies are purely theoretical.

The recent developments in additive manufacturing techniques have made it possible to fabricate and develop unconventional structures, such as metamaterials [25]. Unfortunately, most of the existing research efforts are limited in the theoretical level, because of the difficulties in manufacturing such materials [26]. Furthermore, the kinematics of deformation of the resulting metamaterial can be measured or tracked through modern full-field methods such as Digital Image Correlation (DIC).

In this work the authors aim to present a review of the theoretical principles that allow the completion of an engineering-cycle for developing anepectic metamaterials. For that purpose, this paper is outlined as follows. In Section 2 important fundamentals about multi-material topology optimization are summarized. The FE models generated to simulate the anepectic behavior as a proof-of-concept are presented in Section 3. In Section 4 are presented fundamentals about multi-material additive manufacturing. Finally, Section 5 outlines the conclusion of this work.

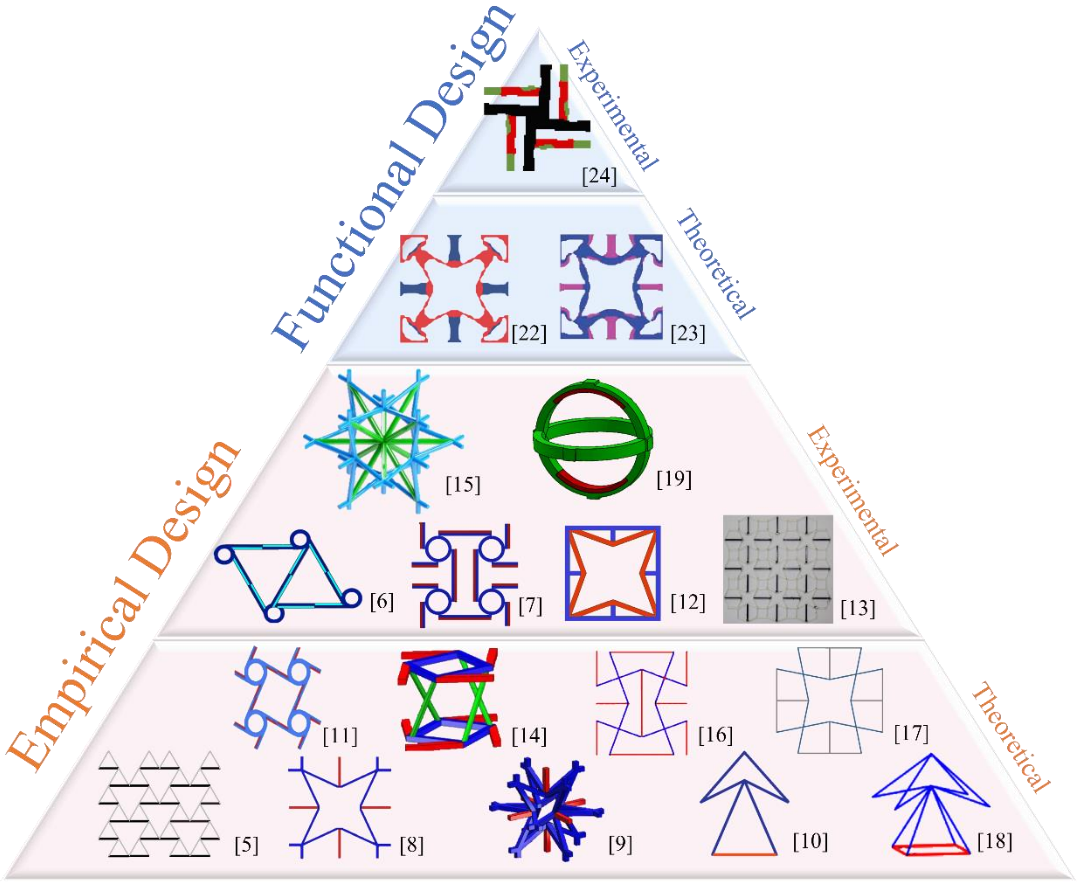


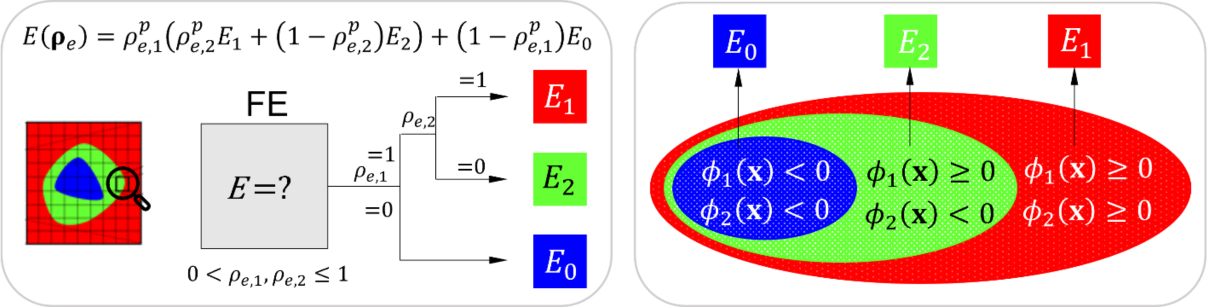
Figure 1: State of the Art of anepectic microstructures, from 2007 to 2022, see each respective reference.

2 MULTI-MATERIAL TOPOLOGY OPTIMIZATION

This section reviews the main theoretical concepts to be considered when optimizing the topology of microstructures to display the anepectic behavior. Firstly, the main optimization approaches are presented. Finally, one considers how to optimize for two objectives.

2.1 Topology Optimization Approaches

Topology optimization may follow different approaches. The most common are the density-based and the level-set approaches. The goal is always to find the optimal material distribution within a predefined design domain [27]. The density-based method uses an artificial density design variable per finite element, ρ_e, and interpolate the material property (e.g., the Young's modulus E) by means of a power-law, as the well-known SIMP. When the artificial density is zero, the material is "void" and when the density is one, the material is "solid". The level set method uses level-set functions, ϕ, to define the optimal structure boundary. When the level set function takes values inferior to one, the material is "void", and superior to one the material is “solid”. Both these methods can be expanded to the multi-material interpolation setting. Figure 2 sketches interpolations according to the different approaches, where E^0, E^1 and E^2 represent the Young’s modulus of the void, material 1 and material 2 phases, respectively.



a) b)

Figure 2: Topology optimization approaches: a) Density-based method and b) Level-set method.

2.2 Multiobjective Topology Optimization

To design anepectic materials, both PR and CTE can be seen as objective functions. Therefore, multiobjective optimization methods are fitting. Multiobjective algorithms, such as Direct Search Method, Genetic Algorithms and Particle Swarm Optimization, deal with both objective functions. However, they are computational expensive for a large number of design variables. A very practical way to deal with multiobjective is to adapt the problem into a single objective function. One can do this by resorting to the well-known weight-sum method, that attributes a weight factor to each objective and then sum them into a single objective function [22]. Another approach is the ε-constraint method, that defines one of the objectives as the problem objective function while the other one is defined as a problem constraint [23].

Consider two arbitrary objective functions, f_ν and f_α, that allow the minimization of the PR and CTE, respectively. Typically, volume constraints are also considered, and other constraints, such as stiffness and symmetry, may also be required.

Using the weight-sum method, the problem is formulated as follows:

$$\begin{aligned} &\min_{\mathbf{x}} w_\nu(\mathbf{x}) f_\nu(\mathbf{x}) + w_\alpha f_\alpha(\mathbf{x}) \\ &s.t. \quad V \leq vf \end{aligned} \tag{1}$$

Where w_ν and w_α are the weight factor associated with the PR and CTE objective function, respectively, vf is the volume fraction and $\mathbf{x}$ are the design variables.

On the other hand, using the ε-constraint method, and considering f_α as the objective function and f_ν as a constraint, the problem is then formulated as follows:

$$\begin{aligned} &\min_{\mathbf{x}} f_\alpha(\mathbf{x}) \\ &s.t. \quad \begin{array}{l} V \leq vf \\ \nu \leq PR^* \end{array} \end{aligned} \tag{2}$$

Where vf is the volume fraction and PR^* is the fixed a *priori* PR negative value.

3 FINITE ELEMENT METHOD

To create a metamaterial FE model, two types of design domains are presented here: A discrete design domain and a continuous design domain. The homogenization theory assumes that the unit-cell is infinitely repeated within the macroscopic domain, however, in practice, a composite material comprises a finite number of repetitions. Here, the convergence of the thermomechanical properties of the two models are evaluated by repeating the unit-cell an increasing number of times [28]. The properties are evaluated at a global and local level, i.e., considering the macrostructure's domain, Ψ, or only the center unit-cell domain, Υ, respectively. For that purpose, only an odd number of repetitions were considered, as presented in Figure 3. Notice that for the unit-cell alone there is no evaluation interest as the micro and macro structures coincide resulting in poor estimate of the metamaterial behavior.

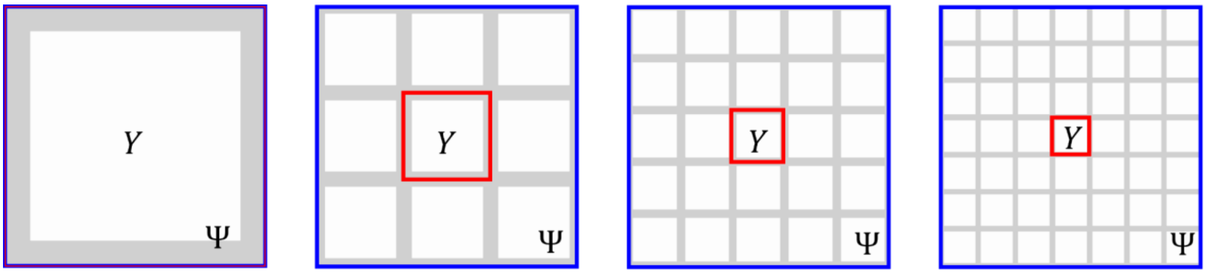
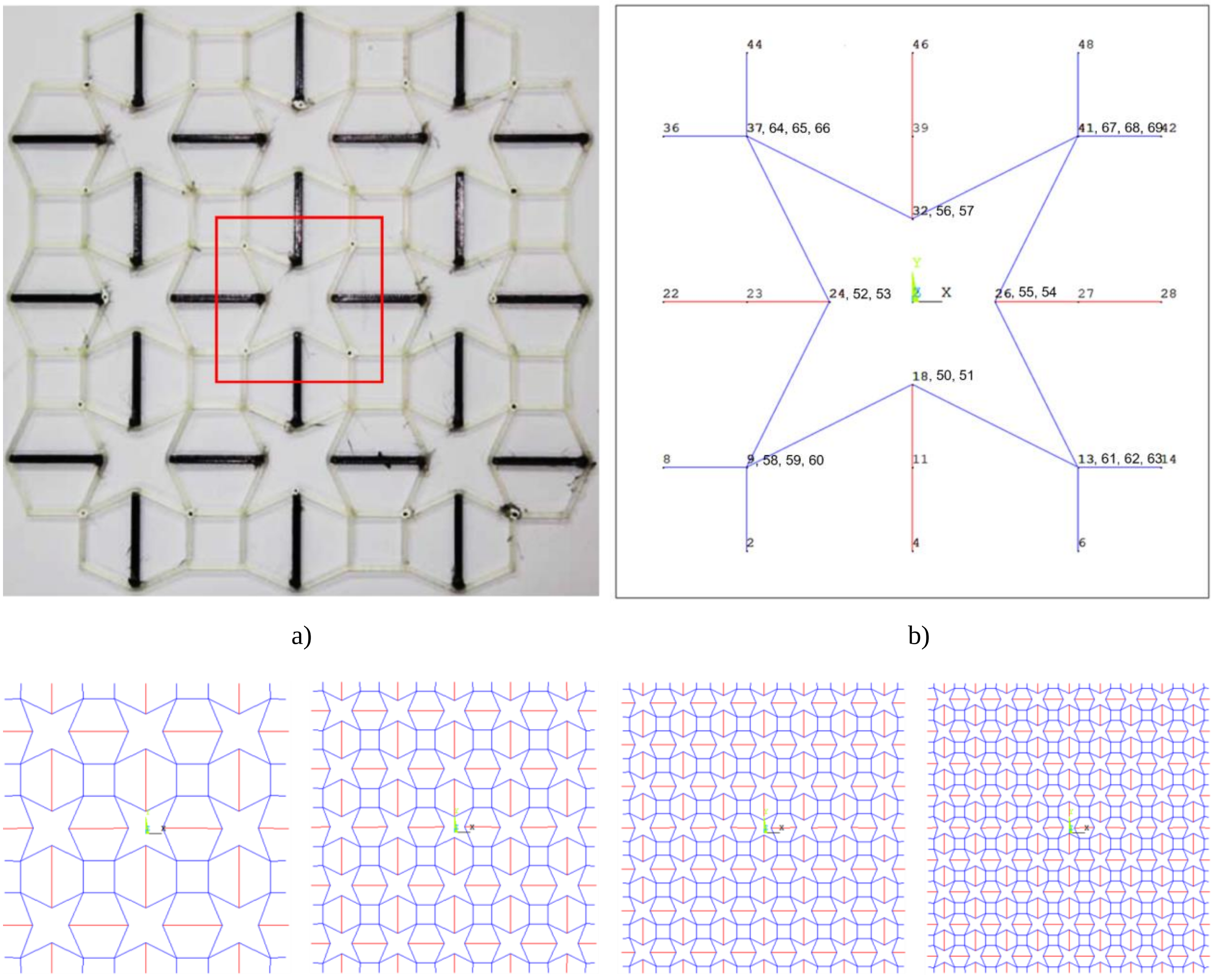


Figure 3: Representation of a macrostructure domain containing *n* x *n* repetitions of the unit-cell. The blue square represents the macroscopic domain, Ψ, and the red square represents the microscopic domain, Υ.

When analyzing the whole domain of the structure, the outer boundary effects (non-periodic) are not negligible. However, when looking at the unit cell domain itself, the deformation is less affected by those effects the more repetitions are considered. This actually renders estimates of metamaterial elastic properties closer to the homogenization predictions. Both evaluations considering the global and local domains to average properties are considered in this framework for comparison purposes. The commercial finite element code ANSYS ® is used to perform the numerical simulations presented in this chapter.

3.1 Discrete Design Domain

In the discrete design domain, the microstructure is discretized using beam elements (BEAM188). However, when using beam elements, the rotation degree of freedom is coupled at each node, unlike bar or link finite elements. To better simulate the deformation mechanism, a torsional spring-type element (COMBIN14) is used at the model joints. This allows to decouple the rotational degree of freedom between two beam elements that share the same node and, consequently, rotational stiffness control at the shared node becomes possible. The FE model developed is based on the metamaterial fabricated in [13] and is presented in Figure 4. The different colors, red and blue, represent different materials, nylon and PVA, respectively.



a)

b)

c)

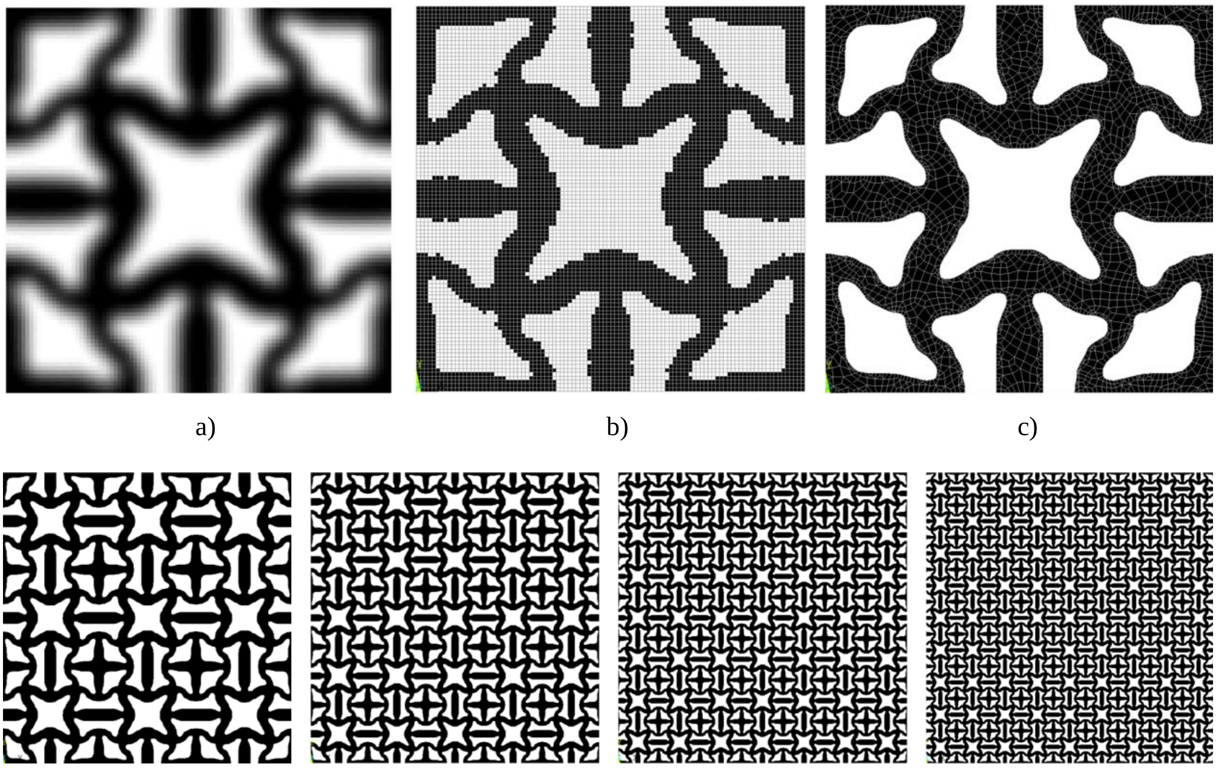
Figure 4: a) Fabricated anepectic mesh in [13] and b) respective unit-cell model. c) FE model with 3×3, 5×5, 7×7 and 9×9 repetitions of the UC.

Symmetry conditions were applied in all simulations. To evaluate the PR a vertical strain of 10% is imposed on the top edge´s nodes while the vertical displacement at the bottom edge’s nodes is constrained. As for the numerical simulation for the CTE, both top and bottom edge’s nodes are constrained and a temperature increment of 93ºC is applied. In both cases the PR and CTE in the horizontal direction are measured based on the horizontal displacements.

It is then verified that the structure exhibits both NPR and NTE. The properties measured locally, i.e., at the unit cell level, converge after three repetitions, however, global properties converge after around seven repetitions. When analyzing the whole domain of the structure, the non-periodic outer BC’s impact on the property value explaining larger deviations from the homogenized property, which is mitigated as the number of repetitions increase. Comprehensively, when looking at the unit cell domain only, the property value for an inferior number of repetitions is less affected by the macroscale boundary effects, resulting in a more accurate measurement toward the homogenized values which were not yet calculated in the scope of the present work for this truss like design.

3.2 Continuous Design Domain

For the continuous design domain, the FE model is based on an optimal auxetic microstructure, designed via the educational Matlab code in [29]. Although TO is a discrete problem, i.e., the so-called “black and white design”, the use of filtering techniques creates areas of intermediate densities, represented by the gray transitions in Figure 5a). The unit-cell extracted from the TO result comprises a mesh of 100×100 4-node quadrilateral elements (PLANE182), shown in Figure 5b), where intermediate densities were not considered. However, the density-based approach results in jagged boundaries which demands proper smoothening. Therefore, to enable the manufacture of the structure, the boundary contour was smoothed resorting to Blender ® software, as shown in Figure 5c).

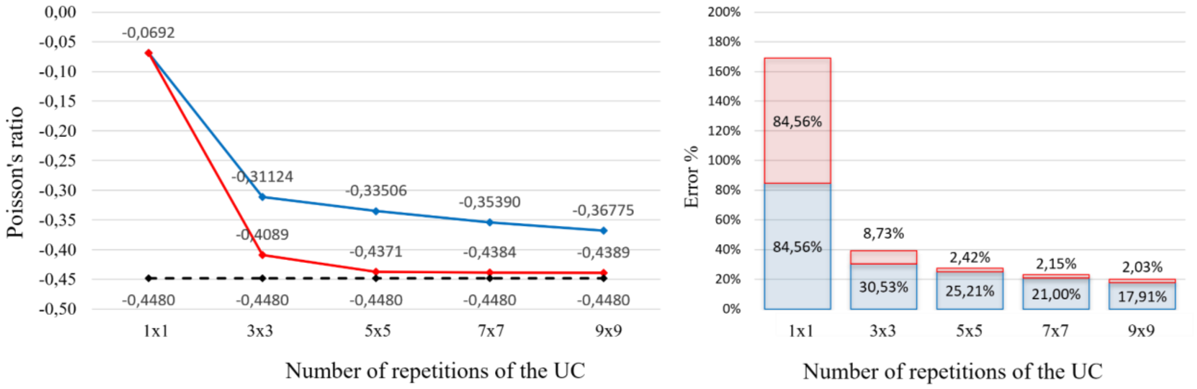

a) b) c)

d)

Figure 5: a) Optimal auxetic microstructure from [29], b) density-based unit-cell model and c) smoothed unit-cell model. d) FE model with 3×3, 5×5, 7×7 and 9×9 repetitions of the smoothed UC.

Despite the design in Figure 5 doesn’t present anepectic behavior, only negative PR, the modelling and analysis just described for this microstructure serves as proof-of-concept as regards translating optimal topology design into manufacturing.

Similar to the discrete domain, a vertical strain is imposed to evaluate the Poisson's ratio in this last model. As shown in Figure 6, as the number of repetitions of the unit-cell increases, the PR of the composite material converges to the homogenized value, which is known running the code in [29]. As expected, the local average is more accurate when compared to the homogenization prediction. Furthermore, it is also verified that considering the FEA of the unit-cell alone that does not illustrate the behavior of the composite material.



a) b)

Figure 6: a) Scale-size effects on the PR. The blue and red lines represent the global and local average, respectively. The dashed black line represents the homogenized Poisson's ratio. b) Error between the homogenization prediction and the FE analyses for the different number of repetitions.

4 ADDITIVE MANUFACTURING AND TESTING

To produce the structures via AM, an Ultimaker 3 was used, along with the software Ultimaker Cura (Updated to the most recent version) to slice the .stl into a .gcode file. This was the same printer and software used in [13]. As a first resort, polylactic acid polymer (PLA) was used due to its easiness to work.

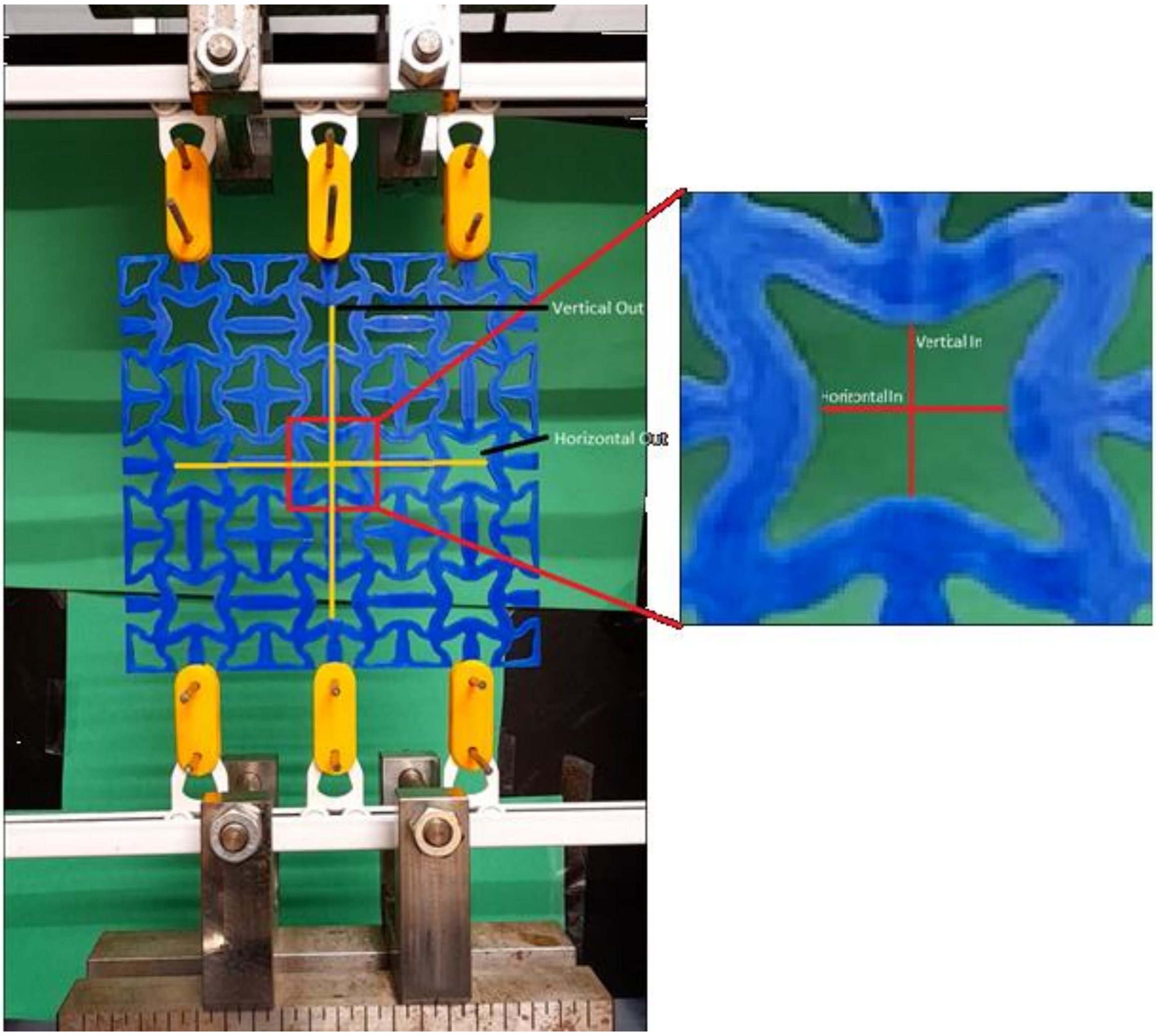
The standard configurations were used with the following exceptions:

1. All layers were printed equally to avoid any gradients in the print direction.
2. The infill was 100% with a cross pattern.
3. Brim was removed.

Mechanical tests were performed with a Shimadzu AG 50kNGT universal testing machine. All tests were performed at a speed of 1 mm/min. A special support was created for stress testing the printed structures. This support allows the horizontal displacements to be as unconstrained as possible, while a vertical strain is applied. The experimental setup is shown in Figure 7a).

To determine the Poisson's ratio of the printed structure, the mechanical tests were filmed, and the software Image-J was used to determine the structure deformation. The vertical and horizontal displacements were measured considering the interior of the central unit-cell, as shown in Figure 7b).

So far, preliminary testing is ongoing and in a near future the authors aim to compare the results with the FE model.



a) b)

Figure 7: a) Experimental setup and b) vertical and horizontal displacements considered.

12 CONCLUSIONS

Metamaterials have been extensively studied in recent decades. However, anepectic solutions, i.e., coupling both NPR and NTE, are still scarce, and even fewer regarding experimental validation. Out of these contributions, only a small percentage takes advantage of the design freedom provided by TO. To develop an optimization formulation capable of dealing with both negative indexes several challenges must be overcome, such as dealing with multi-objective and multi-material formulations. As for the fabrication of anepectic metamaterials, the major challenge lies in producing multi-material structures with complex geometries that require specific machinery. Also, when performing both the computational and experimental analysis, both models must be tuned, i.e., one must choose the adequate FE and BC's that will replicate the experimental tests. The unresolved issues and challenges discussed above can offer great opportunities for further studies and development of anepectic metamaterials.

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REFERENCES

[1] Huang, C. and Chen, L. Negative Poisson's Ratio in Modern Functional Materials. *Adv. Mater.*, (2016) **28**:8079-8096.

[2] Ren, X., Das, R., Tran, P., Ngo, T.D. and Xie, M. Auxetic metamaterials and structures: a review. *Smart Mater. Struct.*, (2018) **27**:023001.

[3] Cardoso, O.J., Borges, J.P. and Velhinho, A. Structural metamaterials with negative mechanical/thermomechanical indices: A review. *Prog. Nat. Sci: Mater Int.,* (2021) **31**:801-808.

[4] Osanov, M. and Guest, J.K. Topology Optimization for Architected Materials Design. *Annu. Rev. Mater. Res.*, (2016) **46**:211-233.

[5] Grima, J.N., Farrugia, P.S., Gatt, R. and Zammit, V. Connected triangles exhibiting negative Poisson's ratio and negative thermal expansion. *J. Phys. Soc. Jpn.*, (2007) **76**:025001.

[6] Ha, C.S., Hestekin, E., Li, J., Plesha, M.E. and Lakes, R.S. Controllable thermal expansion of large magnitude in chiral negative Poisson's ratio lattices. *Phys. Status Solidi B*, (2015) **252**:1421-1434.

[7] Wu, L., Li, B. and Zhou, J. Isotropic Negative Thermal Expansion Metamaterials. *ACS Appl. Mater. Interfaces*, (2016) **8**:17721-17727.

[8] Ai, L. and Gao, X.-L. Metamaterials with negative Poisson's ratio and non-positive thermal expansion. *Compos. Struct.*, (2017) **162**:70-84.

[9] Ai, L. and Gao, X.-L. Three-dimensional metamaterials with a negative Poisson's ratio and a non-positive coefficient of thermal expansion. *Int J. Mech. Sci.*, (2018) **135**:101-113.

[10] Wei, K., Peng, Y., Qu, Z., Pei, Y. and Fang, D. A cellular metastructure incorporating coupled negative thermal expansion and negative Poisson's ratio. *Int. J. Solids Struct.*, (2018) **150**:255-267.

[11] Yu, H., Wu, W., Zhang, J., Chen, J., Liao, H. and Fang, D. Drastic tailorable thermal expansion chiral planar and cylindrical shell structures explored with finite element simulation. *Compos. Struct.*, (2019) **210**:327-338.

[12] Li, X., Gao, L., Zhou, W., Wang, Y. and Lu, Y. Novel 2D metamaterials with negative Poisson's ratio and negative thermal expansion. *Extreme Mech. Lett.*, (2019) **30**:100498

[13] Raminhos, J.S., Borges, J.P and Velhinho, A. Development of polymeric anepectic meshes: auxetic metamaterials with negative thermal expansion. *Smart Mater. Struct.*, (2019) **28**:045010

[14] Fu, M., Huang, J., Zheng, B., Chen, Y. and Huang, C. Three-dimensional auxetic materials with controllable thermal expansion. *Smart Mater. Struct.* (2020) **29**:085034.

[15] Yazdani Sarvestani, H., Akbarzadeh, A.H., Therriault, D. and Lévesque, M. Engineered

Bi-material Lattices with Thermo-mechanical Programmability. *Compos. Struct.*, (2021) **263**:113705.

[16] Li, J., Yang, Q., Wei, Y., Huang, N. and Tao, R. A synergistic design of composite metamaterial with drastically tailorable thermal expansion and Poisson's ratio. *Compos. Struct.*, (2021) **275**:114446.

[17] Peng, X.-L. and Bargmann, S. A novel hybrid-honeycomb structure Enhanced stiffness, tunable auxeticity and negative thermal expansion. *Int J. Mech. Sci.*, (2021) **190**:106021.

[18] Peng, Y., Wei, K., Mei, M., Yang, X. and Fang, D. Simultaneously program thermal expansion and Poisson's ratio in three dimensional mechanical metamaterial. *Compos. Struct.*, (2021) **262**:113365.

[19] Gonçalo M. R. Catatão, M.Sc. thesis, *Additive Manufacturing and Characterization of Three-dimensional Anepectic Structures*, Universidade Nova de Lisboa, 2020/2021.

[20] Sigmund, O. Materials with prescribed constitutive parameters: An inverse homogenization problem. *Int. J. Solids Structures*, (1994) **31**:2313-2329.

[21] Sigmund, O. and Torquato, S. Design of materials with extreme thermal expansion using a three-phase topology optimization method. *J. Mech. Phys. Solids.*, (1997) **45**:1037-1067.

[22] Wang, Y., Gao, J., Luo, Z., Brown, T. and Zhang, N. Level-set topology optimization for multimaterial and multifunctional mechanical metamaterials. *Engineering Optimization*, (2017) **49**:22-42.

[23] Vineyard, E. and Gao, X.L. Topology and Shape Optimization of 2-D and 3-D Micro-Architectured Thermoelastic Metamaterials Using a Parametric Level Set Method. *CMES-Computer Modeling in Engineering & Sciences*, (2021) **127**:819-854.

[24] Han, Z. and Wei, K. Multi-material topology optimization and additive manufacturing for metamaterials incorporating double negative indexes of Poisson's Ratio and thermal expansion. *Additive Manufacturing*, (2022) **54**:102742.

[25] Joseph, A., Mahesh, V. and Harursampath, D. On the application of additive manufacturing methods for auxetic structures: a review. *Adv. Manuf*, (2021) **9**:342-368.

[26] Wu, X., Su, Y. and Shi, J. Perspective of additive manufacturing for metamaterials development. *Smart Mater. Struct.* (2019) **28**:093001.

[27] Sigmund, O. and Maute, K. Topology optimization approaches. *Struct Multidis Optim*, (2013) **48**:1031-1055.

[28] Coelho, P.G., Amiano, L.D., Guedes, J.M. and Rodrigues, H.C. Scale-size effects analysis of optimal periodic material microstructures design by the inverse homogenization method. *Comput. Struct.*, (2016) **174**:21-32.

[29] Xia, L. and Breitkopf, P. Design of materials using topology optimization and energy-based homogenization approach in Matlab. *Struct Multidis Optim*, (2015) **52**:1229-1241