This thesis has been submitted in fulfilment of the requirements for a postgraduate degree (e. g. PhD, MPhil, DClinPsychol) at the University of Edinburgh. Please note the following terms and conditions of use:

- This work is protected by copyright and other intellectual property rights, which are retained by the thesis author, unless otherwise stated.
- A copy can be downloaded for personal non-commercial research or study, without prior permission or charge.
- This thesis cannot be reproduced or quoted extensively from without first obtaining permission in writing from the author.
- The content must not be changed in any way or sold commercially in any format or medium without the formal permission of the author.
- When referring to this work, full bibliographic details including the author, title, awarding institution and date of the thesis must be given.
From 4-dimensional polytope projections to a new class of 3D printed mechanical metamaterials

Thesis submitted in fulfilment of

of

Doctor of Philosophy

by

Gabrielis Černiauskas

THE UNIVERSITY
of EDINBURGH

School of Engineering
Institute for Materials and Processes
The University of Edinburgh
July 2023
Abstract

In order to reduce carbon emissions from transportation and renewable energy sectors, there has been an increasing interest in the development of high-performance lightweight materials. Metamaterials are an example as their artificially engineered geometries exhibit unusual properties that can outperform natural materials. The recent advancements in digital manufacturing approaches, such as additive manufacturing, have enabled the fabrication of metamaterials with increasingly complex geometrical arrangements favouring the resultant mechanical properties.

Metamaterial designs based on hierarchical structures were shown to be advantageous for stiffness and strength applications. While the mathematical concept of closed 4-dimensional geometrical objects (i.e. 4-polytopes) have geometrical similarities to hierarchical designs, this has not yet been explored in the emerging field of mechanical metamaterials. In this work, the 3D projections of 4-polytope geometries are investigated for mechanical applications which require high specific stiffness and strength under compressive, tensile and shear loading conditions.

Using computational modelling and evolutionary optimisation algorithms, this work outputs a new class of mechanical metamaterials which include 5-cell, 8-cell, 16-cell and 24-cell designs. The performance of this class was simulated using finite element analysis and also mechanically characterised and validated using additively manufactured samples. The cubically symmetrical metamaterials were benchmarked against commonly researched structures including the gyroid and hexagonal honeycomb. The knowledge gathered throughout this research was summarised as guidelines for future mechanical metamaterial design.

The results from this work prove the potential of 4-polytopes in mechanical metamaterial design, opening a new avenue of research in the field. Further research and validation of these highly customised and lightweight metamaterials are expected to benefit different sectors of engineering including transportation, aerospace and energy applications.
Lay summary

In order to reduce carbon emissions from transportation and renewable energy sectors, there has been an increasing interest in the development of new lightweight materials that have exceptional mechanical properties. Currently, various types of solid materials, such as plastics, metal alloys and composite materials, are commonly used for high-end applications. The performance of these materials can be enhanced even further by introducing an ordered arrangement of tiny holes or spaces to the material block which makes the material lighter without losing its effectiveness.

Metamaterials are an example of such materials that are carefully designed to have unique properties. They are engineered to have an ordered arrangement of cavities within the solid in a way that is different from how materials are usually found in nature. The presence of cavities forms geometrical structures that exhibit enhanced or even unusual properties which are rarely achieved using solid materials. The recent advancements in digital manufacturing approaches have enabled the fabrication of these structures. Metamaterials with increasingly complex internal geometries favouring the resulting mechanical and physical characteristics can now be manufactured using 3D printing.

Previous research in the field has demonstrated that metamaterials designed using a layered arrangement of structures, also called hierarchical structures, are beneficial for stiffness and strength applications. While the mathematical concept of closed 4-dimensional geometrical objects (i.e. 4-polytopes) have geometrical similarities to hierarchical structures, this has not yet been explored in the emerging field of mechanical metamaterials. In this work, 4-polytopes are represented as 3-dimensional structures and are then used for the development of lightweight, stiff and strong metamaterials. The geometric projection approach is used as a dimensionality reduction technique to enable the representation of 4-polytopes in 3-dimensional space. Three loading cases are investigated, namely compression, tension and shear, when assessing the metamaterial samples. Due to the inherited geometrical features of 4-polytopes, the developed metamaterials have the same mechanical properties along the three perpendicular axes of each sample.
Using computational modelling and evolutionary optimisation algorithms, this work outputs a new class of mechanical metamaterials which include 5-cell, 8-cell, 16-cell and 24-cell designs. The performance of this class was simulated using finite element modelling and also mechanically tested and validated using 3D printed samples. The new metamaterials were also benchmarked against commonly researched structures including the gyroid and hexagonal honeycomb. The knowledge gathered throughout this research was summarised as guidelines for future mechanical metamaterial design.

The results from this work prove the potential of 4-polytopes in mechanical metamaterial design, opening a new avenue of research in the field. Further research and validation of these highly customised and lightweight metamaterials are expected to benefit the different sectors of engineering including transportation, aerospace and energy applications.
Acknowledgements

Thanks to my supervisor Dr Parvez Alam for all of his contributions to my work and professional development. It has been a real pleasure working with him as he is one of the most positive and supportive people I have ever met. Regardless of the conversation topic, I’d always leave our meetings with a smile on my face.

I am also grateful to everyone else who contributed to my project through our formal and informal discussions. I sincerely thank Prof Frank Mill, Dr Colin Robert and Prof Conchúr Ó Brádaigh for their insightful input. Many thanks to Donal O’Flynn for the opportunity to collaborate on the design of wind turbine blades and for giving me the chance to apply the skills I developed during this PhD to a real-world problem. Lastly, thanks to my colleagues and friends in the Composites group at IMP.

My special thanks go out to my family for their love and support throughout this journey. To my one and only Desen who kept me going and reminded me of the beauty of life when the times got tough, mersi çok dâdım!
Declaration

I declare that the work presented in this thesis has been composed solely by myself and that it has not been submitted, either in whole or in part, in any previous application for a degree. Except where otherwise acknowledged, the work presented is entirely my own.

Gabrielis Ėerniauskas

July 2023
Contents

1 Introduction and background ................................. 1
  1.1 Background to the research .............................. 1
  1.2 Mechanical metamaterials ................................. 2
  1.3 Significance of mechanical metamaterial research .......... 3
  1.4 Application of polytope concepts in mechanical metamaterial design . 4
  1.5 Research problem ........................................... 5
  1.6 Hypothesis statement ...................................... 6
  1.7 Summary of key findings .................................... 6
  1.8 Structure of the thesis .................................... 7
  1.9 Research dissemination .................................... 10

2 Literature Review ............................................. 12
  2.1 Mechanical metamaterials ................................. 12
    2.1.1 Enhancing stiffness and lightweightness ............... 14
    2.1.2 Lattice structures ..................................... 16
    2.1.3 Thin-walled structures .................................. 18
    2.1.4 Minimal surface structures ............................... 20
    2.1.5 Shear stiff structures ................................... 22
  2.2 4-polytope-based structures: a new class of mechanical metamaterials 23
    2.2.1 Regular and convex polytopes ............................ 23
    2.2.2 Schlegel diagram ........................................ 24
    2.2.3 4-polytope applications in mechanical metamaterials .......... 26
  2.3 Optimisation and computational design ...................... 28
    2.3.1 AI and nature-inspired optimisation algorithms ........... 28
    2.3.2 Parametric optimisation of mechanical metamaterials .......... 30
      2.3.2.1 Genetic algorithm .................................... 31
3 Methods for designing, optimising, manufacturing and testing 4-polytope-based metamaterials

3.1 Design of 4-polytope-based structures ........................................ 37
    3.1.1 Unit cell design ..................................................... 37
    3.1.2 Stacking of unit cells ............................................. 41
3.2 Unit cell simulations .......................................................... 45
    3.2.1 Boundary conditions for the compression set ....................... 47
    3.2.2 Boundary conditions for the tension set ............................ 47
    3.2.3 Boundary conditions for the shear set ............................. 49
3.3 Parametric optimisation ..................................................... 50
3.4 Manufacturing ................................................................. 54
    3.4.1 Compression sample manufacturing ................................. 55
    3.4.2 Tension sample manufacturing ...................................... 57
    3.4.3 Shear sample manufacturing ....................................... 59
3.5 Mechanical testing ......................................................... 60
    3.5.1 Compressive testing set up ....................................... 60
    3.5.2 Tensile testing set up ............................................ 61
    3.5.3 Shear testing set up ............................................... 62

4 Properties of the compressive metamaterial set .................................. 63

4.1 Simulation results ........................................................... 63
4.2 Experimental testing results ................................................ 66
    4.2.1 Specific stiffness and yield strength properties .................. 66
    4.2.2 Effect of optimisation on other mechanical properties .......... 70
    4.2.3 Performance comparison with existing mechanical metamaterials 74
4.3 Key findings ................................................................. 77
5 Properties of the tensile metamaterial set
  5.1 Simulation results ............................................... 79
  5.2 Experimental results ............................................ 82
    5.2.1 Specific stiffness and yield strength properties ........... 82
    5.2.2 Effect of optimisation on other mechanical properties ..... 89
    5.2.3 Performance comparison with existing mechanical metamaterials 91
  5.3 Key findings .................................................... 95

6 Properties of the shear metamaterial set
  6.1 Simulation results ............................................... 97
  6.2 Experimental results ............................................ 101
    6.2.1 Specific shear stiffness and shear yield strength properties . 101
    6.2.2 Effect of optimisation on other mechanical properties ..... 108
    6.2.3 Performance comparison with existing mechanical metamaterials110
  6.3 Key findings .................................................... 113

7 Comparison and evaluation of the optimised metamaterial sets 115
  7.1 Comparison of the unit cell sets developed for compression, tension
      and shear ......................................................... 115
  7.2 Limitations and mitigation strategies ........................... 119
    7.2.1 Simulation related limitations .................................. 119
    7.2.2 Optimisation related limitations ................................ 121
    7.2.3 Manufacturing associated limitations .......................... 121
    7.2.4 Mechanical testing associated limitations ....................... 123
  7.3 Design simplifications for future work ........................ 124
  7.4 Emerging application and challenges for mechanical metamaterials . 126

8 Conclusions 130
  8.1 Validation of the thesis statement ............................. 130
  8.2 Summary of the key findings .................................... 130
  8.3 Implications of the research ................................... 131
  8.4 Final remarks .................................................. 132

A Parametric design variables 134

B Progressive optimisation outputs 138
## List of Figures

1.1 Examples of 3D metamaterial structures: (a) a 3D voronoi structure, image adapted from [1], (b) an octet-truss lattice structure [2] and (c) a triply periodic minimal surface (TPMS) structure - a gyroid [3]. . . 3

1.2 Classification of polytopes: 2-dimensional polygon (2-polytope), 3-dimensional polyhedron (3-polytope) and 4-dimensional polychoron (4-polytope). ................................................................. 4

1.3 Structure of the thesis outlining the relationship between the chapters. 8

2.1 Classification of mechanical metamaterials by their enhanced properties, following the methodology presented in [4]. ......................... 13

2.2 Examples of stretch-dominated (in blue) and bending-dominated (in green) 3D structures. The representations are adapted from [5, 6, 7, 8]. 17

2.3 Examples of stretch-dominated thin-walled geometries in 3D (in red) and in 2D (in yellow). The representations are adapted from [5, 9, 10, 11]. 19

2.4 Examples of triply periodic minimal surface structures. The representations are adapted from [12, 13]. ................................. 21

2.5 An illustration of (a) two sets of polygons (squares) in 2D space arranged around a vertex (in red). These sets are then (b) “pushed” into a 3D space to (c) form a polyhedron (cube). ......................... 24

2.6 A diagram illustrating a projection of a cube (a 3D geometry) to 2D space. The formed image in blue is a Schlegel diagram of a cube. . . 25

2.7 Examples of regular 4-polytopes shown as 3D wireframes. The dashed line identifies the four wireframes further analysed in this thesis. . . 26

2.8 Increasing trend of different AI-based and nature-inspired techniques in mechanical metamaterial design. ........................................... 29
2.9 Three examples of industry applications which include (a) meta-implants (hip stems) [14], (b) morphing airfoils [15] and (c) high-end athletic footwear [16].

3.1 Wireframe Schlegel diagrams (perspective projection) of regular convex 4-polytopes (top) and the 4-polytope-based structures designed using the wireframe diagrams (bottom).

3.2 Parametric design approach to 4-polytope-based metamaterial design. Adjustable parameters are marked in letters for each structure.

3.3 Schematic representation of a stacking arrangement using the linear pattern where (a) illustrates it along the two axes, which are marked as Direction X and Direction Z, (b) shows the staking along direction X, (c) displays it along both X and Z directions and (d) represents the top view of the resultant metamaterial array.

3.4 Schematic representation stacking using a mirroring pattern. Where (a) shows the mirroring planes X and Z, (b) displays the mirrored cell across plane X, (c) shows it across both X and Z and (d) represents the top view of the resultant metamaterial array.

3.5 Schematic representation of unit cell stacking approach. The cells shown in colour illustrate the smallest repeated arrangement in each metamaterial case while the shaded areas depict the repetition in the stacking pattern. The markings in red show the interface surfaces between the neighbouring unit cells.

3.6 Boundary conditions of FEA models for 5, 8, 16, 24-cell metamaterial cells (top) and equivalent 4-polytope-based unit cells (bottom). The outer surfaces of a unit cell were prescribed symmetry boundary conditions about the X and Z planes located at the interface between the two adjacent cells. A quarter of each unit cell was modelled by using the internal symmetry planes which are marked in yellow (symmetry about a plane Z) and black (symmetry about a plane X) dashed lines with encastre boundary condition at the bottom and a compressive displacement at the top of the cell.
3.7 Summary of the boundary conditions applied to 4-polytope-based metamaterial quarter unit cell models (left side) and the full cell illustrations (right side). The outer surfaces of each model were prescribed symmetry boundary conditions about the X and Z planes located at the interface between the neighbouring cells. Orange and red dashed lines on the quarter models (left side) mark the inner X and Z symmetry planes within the unit cells respectively which were prescribed symmetry boundary conditions. An encastre BC was used at the bottom and a tensile displacement BC at the top of each quarter model.

3.8 Summary of the boundary conditions applied to the unit cells developed for the shear set loading conditions. A full unit cell was simulated with the two X planes (marked in yellow dashed line) representing the periodic boundary conditions, while the bottom and the top of the cell are prescribed an encastre and a shear loading condition respectively. For each unit cell, the top view (left) and the perspective view (right) are shown.

3.9 Schematic representation of genetic algorithm used in the optimisation framework.

3.10 Representative compressive test specimens with a $5 \times 5 \times 5$ 3D projected 4-polytope unit cell array: (a) 5-cell, (b) 8-cell, (c) 16-cell and (d) 24-cell, and additional structures used as ‘comparative experimental controls’ also in a $5 \times 5 \times 5$ array: (e) gyroid and (f) hexagonal honeycomb (tested in the out-of-plane direction).

3.11 Tensile specimen geometry designed to recreate the tensile behaviour of a “dog bone” shape coupon (black solid line). Main specimen areas: gripping (in purple), transition structure (in orange) and dedicated test unit cells (red dashed line).

3.12 Representative tensile test specimens with a $2 \times 2 \times 4$ 3D projected 4-polytope unit cell array. From left to right: 5-cell, 8-cell, 16-cell and 24-cell, and additional structures used as ‘comparative experimental controls’ - gyroid and hexagonal honeycomb (tested in the out-of-plane direction).
3.13 Representative shear test specimens with a $2 \times 2 \times 8$ 3D projected 4-polytope unit cell array. From left to right, 5-cell, 8-cell, 16-cell and 24-cell, and additional structures used as ‘comparative experimental controls’ - gyroid and hexagonal honeycomb.

3.14 Two vertical strain measurements were taken across the flat features in the same plane, located at the outermost surfaces of the specimen in the middle of the $5 \times 5$ metamaterial cell array ((a)–(d)). Similarly, the strains of the hexagonal honeycomb (e) and gyroid (f) were measured using the flat outermost surfaces and flat features on these surfaces. The strain values (strain 1 & strain 2) were averaged to obtain the overall strain of a specimen. The same strain measurement approach was used for tension and shear metamaterial sets.

4.1 Increases in specific stiffness with incremental optimisation progression from the unoptimised (0%) to the fully-optimised (100%) iteration for 24, 16, 5 and 8-cell metamaterial structures, in that order.

4.2 Comparison of optimised 4-polytope-based structure models with labels (i) to (iv) representing optimisation level: 0% (unoptimised), 33%, 67% and 100% (fully-optimised) structures, respectively. The colour map shows the elastic strain energy density (ESEDEN) distribution in J/cm$^3$ at the compression strain of 0.08 in each structure.

4.3 Comparison of experimental results of 4-polytope-based metamaterials to honeycomb and gyroid structures ($n = 5$).

4.4 Upper and lower experimental bound stress-strain curves, and simulation stress-strain curves for 5-cell, 8-cell, 16-cell and 24-cell 4-polytope-based structures.

4.5 Representative compressive stress-strain curves for each of the experimental sample sets (3D projected 4-polytopes, gyroids and hexagonal honeycombs).

4.6 The compressive strength normalised by bulk Young’s modulus plotted against the relative density of the sample - the data points are plotted against generalised area plots for different metamaterial structures at the nano, micro and macro length scales.
5.1 Specific stiffness comparisons between the 5, 8, 16 and 24-cell 3D projected 4-polytopes from unoptimised (0%) to fully optimised (100%) showing 25% increments of progression in the optimisation process.  

5.2 Color maps for each of the 3D projected 4-polytope metamaterials. Each column illustrates the progress in optimisation at the following different stages: (i) 0% (unoptimised), (ii) 25%, (iii) 50%, (iv) 75% and (v) 100% (fully optimised). The colour legend represents the elastic strain energy density (ESEDEN) values in J/cm$^3$ and the cells are loaded in tension to 2% strain.  

5.3 Specific properties plot comparing the experimental results of the 3D projected 4-polytope metamaterials with gyroid and honeycomb structures in tension.  

5.4 Stress-strain plots for 5-cell, 8-cell, 16-cell and 24-cell 4-polytope-based metamaterials. Simulated results of axial stress along the direction of loading (S22) are presented as dashed lines while upper and lower experimental result bounds are shown as solid lines.  

5.5 Experimental results for 4-polytope-based metamaterials, gyroid and honeycomb samples compared against P and G shellular structures [12, 17]. The figure represents (a) normalised Young’s modulus ($E/E_0$) and (b) normalised strength ($\sigma/\sigma_y$) values plotted against relative sample density. G shellular results are only shown in (a), generalised performance indices for honeycombs, foams and natural materials are shown in (a) and (b). All the data for P and G shellular structures and generic performance indices for foams, honeycombs and natural materials were obtained using axial compressive rather than tensile testing. Dashed lines represent scaling laws that are shown for P and G shellular and honeycomb structures based on the methodology and data presented in [3] and [12] respectively.  

5.6 Experimental results for 4-polytope-based metamaterials, gyroid and honeycomb samples showing tensile strength/ Young’s modulus ($\sigma_t/E_0$) performance index plotted against relative sample density. The plot includes scaling law trendlines for each sample set.
6.1 Specific shear stiffness comparison for the 5, 8, 16 and 24-cell polytopes in shear as the optimisation advances from unoptimised (0%) to fully-optimised (100%) state in 25% progression increments.

6.2 Colour maps for each of the 4-polytope-based structures with each column illustrating optimisation progression at a different level: (i) 0% (unoptimised), (ii) 25%, (iii) 50%, (iv) 75% and (v) 100% of total optimisation (fully-optimised) metamaterial unit cells. The colour legend represents a range of elastic strain energy density (ESEDEN) values in J/cm$^3$ when the cells are loaded in shear to 0.10 strain.

6.3 Specific shear properties plot for experimental 4-polytope-based metamaterial samples together with gyroid and honeycomb structures.

6.4 Shear stress-strain curves for 5, 8, 16 and 24-cell metamaterials. Upper and lower experimental bounds are presented in solid lines while simulated results are shown as dashed lines.

6.5 Experimental comparison of 4-polytope-based metamaterials with gyroid, hexagonal honeycomb samples, as well as other metamaterial structures presented in, [18, 19], namely, Kelvin, octet, idealised foam and cubic lattices. The figure presents the results for (a) normalised shear modulus ($G/G_0$) and (b) normalised shear strength ($\tau/\tau_0$) plotted against the relative density. Parts (b) of the figure also include scaling law trendlines for all 4-polytope-based metamaterial structures and gyroid and hexagonal honeycomb samples.

6.6 Shear yield strength over shear modulus ($\tau_y/G_0$) plotted against the relative density for experimental comparison of 4-polytope-based metamaterials with gyroid, hexagonal honeycomb samples. The figure includes scaling law trendlines for all 4-polytope-based metamaterial structures and gyroid and hexagonal honeycomb samples.

7.1 Comparison of the best-performing unit cell structures in all three optimised metamaterial sets, namely, compression (in grey), tension (in blue) and shear (in green). The structures with the highest specific (axial/shear) stiffness values within each set are marked in dashed red while the ones with the highest specific (axial/shear) strength are marked in solid yellow.
7.2 Illustration of inner and outer geometrical features within each 4-polytope-based unit cell. .................................................. 117
7.3 A diagram showing width, breadth and length of the representative samples from each metamaterial set. .............................. 122
7.4 Strengths, weaknesses, opportunities and threats (SWOT) of mechanical metamaterials .................................................. 127

B.1 Progressive optimisation of the compressive metamaterial set with each column showing the geometrical arrangement at a different stage. . . . 139
B.2 Progressive optimisation of the tensile metamaterial set with each column showing the geometrical arrangement at a different stage. . . 140
B.3 Progressive optimisation of the shear metamaterial set with each column showing the geometrical arrangement at a different stage. . . . 141

C.1 Inside Front Cover: Advanced Engineering Materials. .................. 143
List of Tables

2.1 Regular convex 4-polytopes and their respective Schlafli symbols. 24
3.1 Parametric design variables and corresponding descriptions for 5, 8, 16 and 24-cell designs as illustrated in Figure 3.2. 40
3.2 Summary of the parameters used in genetic algorithm set-up. 52
4.1 Mean specific stiffness $\bar{\frac{E}{\rho}}$ results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures and specific stiffness values $\bar{\frac{E}{\rho}}$ for simulated models: 5, 8, 16 and 24-cell metamaterials. 68
4.2 Mean specific yield strength $\bar{\frac{\sigma_y}{\rho}}$ results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures, and specific strength values $\bar{\frac{\sigma_y}{\rho}}$ for simulated models: 5, 8, 16 and 24-cell metamaterials. 69
4.3 Summary of experimentally obtain mechanical properties: Young’s modulus (compression), yield and compressive strength, modulus of resilience and modulus of toughness for 4-polytope-based metamaterials, and for gyroid and hexagonal honeycomb structures. 73
4.4 Apparent and relative densities of simulated and experimentally tested samples. 75
4.5 Calculations of constants $C$ and $D$ using experimental data in Tables 4.3 and 4.4. 76
5.1 Mean specific stiffness $\bar{\frac{E}{\rho}}$ results for experimental 4-polytope-based metamaterial samples (5, 8, 16 and 24-cell) together with gyroid and hexagonal honeycomb results. The experimental results are compared against the simulated specific stiffness $\bar{\frac{E}{\rho}}$ outputs using percentage differences and Z-score values. 85
5.2 Mean specific yield strength $\bar{\sigma}_y$ results for experimental 4-polytope-based metamaterial samples (5, 8, 16 and 24-cell) together with gyroid and hexagonal honeycomb results. The experimental results are compared against simulated specific yield strength $\bar{\sigma}_y$ outputs using percentage differences and Z-score values. ........................................ 86

5.3 Summary of experimentally obtained mechanical properties for 4-polytope-based metamaterials as well as gyroid and hexagonal honeycomb samples. The table presents Young’s modulus, yield and tensile strength and modulus of resilience and toughness values. .............................. 89

5.4 Apparent and relative densities for simulated and experimentally tested samples. The table includes percentage difference values between simulated and experimentally obtained apparent densities. .................. 90

6.1 Mean specific shear stiffness $\bar{G}_\rho$ results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures and specific shear stiffness values $G_{\rho}$ for simulated models: 5, 8, 16 and 24-cell metamaterials. ................................. 104

6.2 Mean specific shear yield strength $\bar{\tau}_y$ results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures, and specific shear strength values $\tau_y$ for simulated models: 5, 8, 16 and 24-cell metamaterials. ................................. 105

6.3 Summary of experimentally obtained mechanical properties: shear modulus, shear yield strength and shear strength, modulus of resilience and modulus of toughness for 4-polytope-based metamaterials, and for gyroid and hexagonal honeycomb structures. ................................. 108

6.4 Apparent and relative densities for simulated and experimentally tested shear samples. ................................................................. 110

A.1 Compression set. Parametric design variable table summarising the specified range used in design space exploration and optimum parameter values (100% of total optimisation - case (iv)) obtained using the optimisation algorithm. The full set of raw optimisation data is also made available on the Edinburgh Data Share website [20]. .......... 135
A.2 Tension set. Parametric design variable table detailing the specified parameter range, starting value and the optimum value obtained using the optimization method (100% of total optimization - case (iv)). The full raw optimization dataset is available on the Edinburgh Data Share website [21].

A.3 Shear set. A list of parametric design variables for each 4-polytope metamaterial including specified parameter range, starting value and the optimum value (100% of total optimization - case (iv)) found using the optimisation algorithm. The full raw optimization dataset is available on the Edinburgh Data Share website [22].
Chapter 1

Introduction and background

1.1 Background to the research

Following the Paris Agreement, numerous countries started transitioning towards a carbon-neutral economy which requires significant technological innovation. As the European Union, the United Kingdom and other countries pledged to reach net zero by 2050, there has been an urge to minimise carbon footprint and reduce greenhouse gas emissions across a wide variety of industries including transport, energy generation and construction. In specific, the transportation sector contributes to 16.2% of worldwide greenhouse gas emissions on its own while the construction and manufacturing sector generates 12.4% [23].

Lightweight high-performance materials, including but not limited to mechanical metamaterials, offer energy-efficient solutions and can act as an enabling factor for reducing the carbon footprint of transportation, construction, renewable energy and various other sectors. Aerospace companies are increasingly using new lightweight components for the purpose of improving fuel efficiency [24]. Similar examples are seen in the electric vehicle market [25] where the use of lightweight composite materials results in lower overall vehicle mass and therefore reduces the overall carbon footprint. Such materials are also used in the development of new wind turbine blades [26] to enable more efficient energy conversion and end-of-life recyclability.

Within the spectrum of lightweight high-performance materials, mechanical metamaterials form a branch with the special ability to design the physical response of a material according to the specified external loading conditions [4]. This is achieved through geometrical manipulation of a metamaterial structure to achieve unusual mechanical and physical properties [6].
Applications of metamaterials range from automotive [27, 28] and aerospace [29, 30] to designing highly customised and high-performance athletic footwear such as Carbon + Adidas collaboration and New Balance [16, 31]. Acknowledging the emerging application areas of mechanical metamaterials, this thesis focuses on designing, manufacturing and testing a new type of mechanical metamaterials which offer superior stiffness, strength and lightweightness in comparison with existing solutions such as lattices, foams, honeycombs and thin-walled structures.

1.2 Mechanical metamaterials

Metamaterials are artificial structures designed to enhance a chosen material property or behaviour which is not usually found in naturally occurring materials [32]. This is achieved through the manipulation of internal substructures to enable a calculated mechanical response that goes beyond the ordinary behaviour of the base material. Although there is a wide range of applications for these engineered materials, this work dwells into metamaterials specifically targeting mechanical property enhancement through geometrical arrangement, otherwise known as “mechanical metamaterials”.

One of the first mentions of mechanical metamaterials is attributed to Lakes [33] who presented foam structures that possess negative Poisson’s ratio in 1987, also known as auxetic metamaterials. Since then, there has been an increasing interest in the development of mechanical metamaterials and the latest wave has been credited to two factors, namely (1) the development of more affordable and widely available additive manufacturing technologies and (2) increasing computational and processing capabilities [34, 35, 36]. This increased our capacity to design and manufacture mechanical metamaterials, which were previously too expensive, complex or cumbersome to produce. Common examples include mechanical metamaterials with auxetic behaviour [32, 37, 38], with tailorable compressive properties [39, 40], with the capacity for high levels of mechanical energy absorption [29, 41] and with high stiffness and strength properties [4, 5, 42, 43].

Mechanical metamaterials are further categorised in terms of their unit cell geometry arrangement into 2-dimensional (2D) and 3-dimensional (3D) metamaterials. The former group includes structures that have unit cell patterns along the 2D plane which is extruded into the 3rd dimension to create thickness to the structure. A few examples include, but are not limited to, multiple variations of honeycombs.
1.3. SIGNIFICANCE OF MECHANICAL METAMATERIAL RESEARCH

such as 2D re-entrant structures [44], diamond [45], triangular [46] and hexagonal honeycombs (most commonly used in industry) [47] and randomly arranged 2D cell structures [48]. The latter group includes the structures which have the geometrical features repeating along the three directions of the metamaterials array. Figure 1.1 shows a few examples of these structures including (a) randomly arranged 3D voronoi structures [1], (b) lattice structures, such as an octet-truss [2], (c) and triply periodic minimal surface (TPMS) structures, such as a gyroid [3]. The work presented in the following chapters of this thesis focuses on 3D mechanical metamaterial structures that have identical unit cells forming 3-dimensional metamaterial arrays.

![Fig 1.1](image-adapted-from-3D-voronoi-structure-octet-truss-gyroid-structures.png)

Figure 1.1: Examples of 3D metamaterial structures: (a) a 3D voronoi structure, image adapted from [1], (b) an octet-truss lattice structure [2] and (c) a triply periodic minimal surface (TPMS) structure - a gyroid [3].

1.3 Significance of mechanical metamaterial research

In addition to the academic research interest highlighted previously, the global market size for lightweight materials and solutions is also increasing. It is forecasted to reach US$230 billion by 2024 with a continued growth rate of 9% [49]. The UK’s Engineering and Physical Sciences Research Council (EPSRC) also encourages research in this area through its “manufacturing the future” theme and the development of mechanical metamaterials directly responds to two of the UK Government’s grand challenges, namely clean growth and future of mobility [50].

3
1.4. APPLICATION OF POLYTOPE CONCEPTS IN MECHANICAL METAMATERIAL DESIGN

Through the combination of academic research, market outlook and the UK’s research strategy presented in this section, it is evident that the emergent field of mechanical metamaterials can provide cascaded benefits through its lightweight and high-performance nature within the automotive, aviation and energy sectors. Therefore, the design, development, manufacturing and testing of optimised mechanical metamaterial structures were pursued as the core part of this thesis.

1.4 Application of polytope concepts in mechanical metamaterial design

This thesis uses the mathematical concepts described in the polytope theory for the design of mechanical metamaterials. A polytope is defined as a geometrical object which possesses flat sides that form faces of this object. In geometrical theory, it can exist in any number of dimensions, however, the most commonly known polytopes are 2D polygons and 3D polyhedra. As shown in Figure 1.2, 4-dimensional (4D) polytopes which are most frequently referred to as 4-polytopes can be visualised in a 3D form through various representation techniques such as Schlegel diagram (described in Section 3.1.1). This project concentrates on exploiting the 3-dimensional geometrical perspectives of 4-dimensional polytopes (i.e. tesseract, simplex) as building blocks for repeatable cells within the metamaterial array.

Figure 1.2: Classification of polytopes: 2-dimensional polygon (2-polytope), 3-dimensional polyhedron (3-polytope) and 4-dimensional polychoron (4-polytope).

While there are a few reports detailing the design of mechanical metamaterials based on hierarchical or fractal substructures [51, 52, 53, 54], 3D projections of 4-
1.5 Research problem

Currently, the use of honeycomb sandwich panels is common for weight reduction. However, structures of this type are mainly designed to carry loads in one direction (i.e. out-of-plane) and have poor in-plane mechanical properties. This stems from the geometry of the hexagonal honeycomb itself and also from the way these structures are manufactured using expansion and corrugation processes. As a result, any significant indentations or faults in the internal geometry or even exposure to
mixed-mode loading (e.g. compression-shear) may lead to the configuration of unstable geometrical equilibrium causing the panel to buckle [61]. With this limitation in mind, this research addresses the development of lightweight metamaterials that have comparable mechanical properties in in-plane and out-of-plane directions, are resilient to geometrical imperfections and are more suited for mixed-loading cases than traditional honeycomb structures.

The reviewed literature shows that metamaterial topologies with hierarchical nature are able to achieve promising mechanical properties, however, the hierarchical arrangements originating from 3D projections of higher dimensional objects have not been addressed in the context of metamaterials. Therefore, there is an obvious gap in knowledge concerning the development of 4-polytope-based (also referred to as 3D projected 4-polytope) mechanical metamaterials, which this thesis aims to address.

The contributions from this work are three-fold as it (1) introduces a new class of mechanical metamaterials, (2) proposes an optimisation framework enhancing the performance of these structures and (3) assesses the mechanical properties of the newly developed metamaterials under three fundamental loading conditions, namely, compression, tension and shear. The work presented herein, to the best of our knowledge, is a pioneer in considering the suitability of 4-polytope projections as base structures for the development of novel mechanical metamaterials.

1.6 Hypothesis statement

A new class of lightweight mechanical metamaterials based on 3D projected 4-polytope geometries can be designed and manufactured to mechanically outperform conventional engineering cellular solids under static loading.

1.7 Summary of key findings

The key findings of the work presented here are summarised as follows:

- 3D projected 4-polytope structures are shown to be highly suitable for the development of a new class of mechanical metamaterials which perform well across a range of different loading conditions, such as compression, tension and shear.
1.8. STRUCTURE OF THE THESIS

- The developed methodology demonstrates that the performance of these structures can be tailored to a specific application and also be significantly enhanced in terms of specific properties related to stiffness and strength by employing an evolutionary algorithm powered optimisation framework.

- The results suggest that 4-polytope-based metamaterials either outperform or perform at a similar level to other commonly researched structures such as the gyroid and hexagonal honeycombs in terms of specific properties related to stiffness and strength in all investigated loading conditions.

- Cubically symmetrical nature of 4-polytope-based mechanical metamaterials provides significant benefits in maintaining structural stiffness and strength when subjected to multi-axial loading which is advantageous in many real-life applications.

- Out of the four 4-polytope-based metamaterial geometries investigated in this work, the 8-cell structures perform the best in terms of specific stiffness and strength in both axial loading scenarios (compression and tension).

- When subjected to shear loading, the 5-cell structure achieves the highest specific shear stiffness and the 8-cell demonstrates the highest specific shear strength properties out of the four 4-polytope-based geometries.

- After comparison of all investigated 4-polytope-based metamaterials, the 8-cell is the top-performing structure under the three modes of static loading: tension, compression and shear.

1.8 Structure of the thesis

This thesis consists of eight chapters with Figure 1.3 presenting the relationship between each of them and also illustrating the overall structure of the thesis.

As Chapters 1 and 2 set the scene for mechanical metamaterial research and discuss the relevant findings in the field, Chapter 3 primarily focuses on the methodology used in this work. Chapters 4, 5 and 6, contribute the most to the technical knowledge of the thesis presenting three sets of 4-polytope-based mechanical metamaterials. Each of these sets is developed for a specific mechanical loading scenario,
1.8. STRUCTURE OF THE THESIS

Figure 1.3: Structure of the thesis outlining the relationship between the chapters.

namely compression, tension and shear in Chapters 4, 5 and 6 respectively. Chapter 7 then compares and analyses the structures developed for the individual loading cases, discusses limitations and mitigation strategies and presents design simplifications of 4-polytope-based structures for future metamaterial design. Finally, Chapter 8 condenses the key research findings, summarises the implications of the research and concludes the thesis.

Below is a brief description of each chapter. Chapter 2 summarises the relevant literature on mechanical metamaterials focusing on motivation, innovative approaches in design methodology and metamaterial applications. The chapter presents the commonly encountered challenges, provides a brief summary of how they are addressed in the literature and demonstrates how computational design approaches aid metamaterial development. It also explains the mathematical theory behind 4-polytopes, discusses how the 4-polytope-based structures are generated and showcases the industrial uses of mechanical metamaterials. Furthermore, the research gaps and op-
opportunities are identified feeding into the key decisions and assumptions of the work presented in the next chapters.

Chapter 3 describes the methodology of this work focusing on the development, modelling and manufacturing of 4-polytope-based mechanical metamaterials. Firstly, it discusses the design of metamaterial unit cells, their stacking arrangements, provides details on simulations and their incorporation into the parametric optimisation framework. Then, it summarises the manufacturing and mechanical testing of metamaterial samples. It also declares the limitations of the methodology and presents the mitigation strategies employed in this work.

Chapter 4 applies the methods presented in the prior chapter for the development of the first set of 4-polytope-based mechanical metamaterials optimised specifically for compressive applications. The chapter summarises results obtained from finite element simulations and experimental testing and compares the newly developed structures against other metamaterials at the nano, micro and macro length scales.

Chapter 5 uses a similar methodology aimed at developing metamaterials resistant to axial loading but focuses on tensile rather than compressive loading presenting new application opportunities for 4-polytope-based metamaterial designs. Similarly to Chapter 4, it demonstrates the specific stiffness and strength properties through simulation and experimental results and also compares the tension set of the 4-polytope-based metamaterials with shellular structures, natural materials and foams.

Chapter 6 explores the suitability of this new class of mechanical metamaterials for another fundamental loading arrangement, namely shear. Specifically, it looks at the specific shear stiffness and shear strength performance of the metamaterial set optimised for this loading condition. The structures are benchmarked against a range of other best-performing metamaterials in shear, once again demonstrating the remarkable mechanical properties of the 4-polytope-based structures.

Chapter 7 then builds on the knowledge presented in Chapters 4, 5 and 6, compares and evaluates the optimised metamaterial sets, discusses limitations and the appropriate mitigation strategies and proposes design simplifications for future work. Additionally, the potential applications and viability of this new class of metamaterials are discussed.
Chapter 8 concludes the research and reiterates the key research findings from the previous chapters. Lastly, the chapter discusses the direct and indirect impact of the research and summarises the thesis.

1.9 Research dissemination

Several research outputs relevant to this work have been produced during the course of this PhD including 7 journal publications, a journal cover, a popular science news article and 3 open-access data sets on 4-polytope-based mechanical metamaterials.

Peer-reviewed journal publications directly related to this thesis:


Other peer-reviewed journal publications:


**Peer-reviewed review articles:**


**Other dissemination:**

- **Inside Front Cover:** *Advanced Engineering Materials*, September 2023 doi: 10.1002/adem.202370058 — (Appendix C)

- “Could marine crabs help us design better helmets?”, 15th Jan 22, *The Curiosity Today Journal*, thecuriositytoday.com/could...helmets

**Open-access data sets:**


Chapter 2

Literature Review

This chapter reviews the key literature in the field of mechanical metamaterials, specifically focusing on the publications relevant to the work presented in this thesis. It surveys the design principles, methodology and results presented in the existing literature discussing their contribution to knowledge. The chapter is divided into three main sections covering mechanical metamaterials associated with high stiffness, strength and lightweightness in Section 2.1, 3D projected 4-polytopes as base structures for mechanical metamaterial design in Section 2.2 and optimisation and computational design methods used for developing and enhancing mechanical metamaterials in Section 2.3. Lastly, it discusses the industrial applications of these artificially engineered structures and details the research gaps that this work aims to address.

2.1 Mechanical metamaterials

Mechanical metamaterials are classified with respect to their response to loading in addition to their geometrical arrangement, as presented in Section 1.2 of Chapter 1. From a modelling perspective, all mechanical metamaterials can be homogenised in the way that the effective properties of a metamaterial structure are represented by an equivalent material block. This allows us to generalise the behaviour of a metamaterial without analysing the response of each individual cell within the array. Following the approach presented in [4], homogenised mechanical metamaterials can be described using the four elastic constants, namely Young’s modulus of elasticity \( E \), Shear modulus \( G \), Bulk modulus \( K \) and Poisson’s ratio \( \nu \). The first three of these constants define the stiffness, rigidity and compressibility of a metamaterial.
2.1. **MECHANICAL METAMATERIALS**

while Poisson’s ratio defines the ratio of transverse to axial strain when metamaterial is loaded axially [4]. As shown in Figure 2.1, comparing mechanical metamaterials using elastic constants allows us to categorise them according to their intended use, namely, to enhance stiffness, alter rigidity and compressibility or achieve auxetic properties.

![Figure 2.1: Classification of mechanical metamaterials by their enhanced properties, following the methodology presented in [4].](image)

The stiffness and lightweightness category, shown in Figure 2.1, includes lattices, thin-walled and minimal surface structures where the rigid structural arrangement of geometrical elements is leveraged to achieve superior stiffness and strength properties. High shear modulus and shear strength structures in the category of rigidity and compressibility are also developed using similar principles. The metamaterials used for achieving high Young’s modulus ($E$) and high shear modulus ($G$) form the main scope of this thesis and a more in-depth literature review is presented in the following sections.

The rigidity and compressibility category also includes, pentamode and kagome structures which, contrary to the shear stiff structures, demonstrate compliant be-
2.1. MECHANICAL METAMATERIALS

haviour. They exhibit a vanishing shear modulus [62], i.e. these are solids that behave like fluids as they are difficult to compress yet easy to deform [63, 64, 65, 66]. This is achieved when the structure has a shear modulus (\(G\)) approaching zero and a finite bulk (\(K\)) modulus, i.e. \(G \ll K\). Hence, the highly rubbery behaviour of pentamode and kagome structures has been found to be useful in a wide range of applications varying from 3D-printed shoes [64] to seismic isolation devices [67]. Lastly, the negative compressibility type in the rigidity and compressibility category, refers to structures which expand in compression or contract in tension [68, 69]. This is achieved when the bulk modulus value for the structure is negative (\(K < 0\)).

The third category shown in Figure 2.1 is on mechanical metamaterials with zero or negative Poisson’s ratio which are referred to as auxetic structures. These structures expand sideways when stretched axially and vice versa. Auxetics are interesting as this behaviour is not seen in monolithic materials such as polymers and metals which have positive Poisson’s ratios [70]. These structures were first proposed by Lakes [33] in 1987 and were shown to gain their auxetic deformation behaviour from the underlying topological arrangement of the structure. They can be further categorised to re-entrant [44], chiral [71], rotating rigid structures [72], and perforated sheet structures [73]. Nevertheless, the auxetic structures are beyond the scope of this work and the following sections of this literature review only focus on passive mechanical metamaterials associated with enhanced stiffness and lightweightness.

2.1.1 Enhancing stiffness and lightweightness

In order to reduce material weight and further decrease the apparent density of any bulk material beyond the density of water, materials must have porosity. This comes at the cost of disproportional reduction of mechanical properties, if the voids are introduced in a random fashion. For example, foams with a relative density (i.e. the volume fraction) of 10% maintain the stiffness and strength that are 0.3% and 0.9% of the constitutive bulk material, respectively [74]. This, however, can be significantly improved by controlling the phase topology of cellular solids where one phase is the void and the other is the constituent material. Several research publications prove [3, 5, 75, 76] that mechanical metamaterial design can achieve superior stiffness-to-weight and strength-to-weight ratios when compared to monolithic bulk materials.

One of the most important concepts in defining whether the mechanical response of a cellular solid is stiff or compliant lies in differentiating between stretch (i.e.
main deformation mechanism is through stretching of the geometrical elements) and bending-dominated (i.e. deformation through bending of geometrical elements) phase topologies [7]. This is assessed by evaluating the relationship between the stiffness and porosity, and the strength and porosity, which for cellular solids tends to follow a power scaling law. It is expressed as $E^* \propto \left(\frac{\rho^*}{\rho_s}\right)^a$ for stiffness and $\sigma^* \propto \left(\frac{\rho^*}{\rho_s}\right)^b$ for strength, where $E$, $\rho$ and $\sigma$ are Young’s modulus, the density and the strength (in non-buckling cases: the yield strength ($\sigma_* = \sigma_y$) for ductile constituent material or the fracture strength ($\sigma_* = \sigma_f$) for brittle material, in buckling cases: elastic buckling strength ($\sigma_* = \sigma_b$)), respectively, with symbol * representing the cellular solid and $s$ indicating the constituent solid material. The work presented by Ashby [7] and Fleck et al. [46] demonstrates that the parameters $a$ and $b$ are equal to 1 for the ideal case of stretch-dominated structures. In contrast, when the phase topology is bending-dominated, the parameter $a$ values range between 2 and 4 while the parameter $b$ can vary between 1.5 and 2 for stochastic structures such as foams [46] and aerogels [77, 78]. These findings, therefore, provide insight into the mechanical behaviour of complex geometrical structures.

The surveyed literature shows that most mechanical metamaterials perform in between the two ends of the spectrum and experience mixed mode deformation [75]. However, the stretch-dominated topologies are more beneficial for lightweight applications having significantly higher stiffness and strength than bending-dominated cellular solids and therefore, are of significance to the work presented in this thesis. This is true even at exceptionally low relative densities that can be achieved with some aerogel and foam solutions as the higher exponent of the power law values ($a$ and $b$ parameters) outweighs the benefits of low apparent density [75]. In other words, the unit cell design must be governed by stretch-dominated behaviour in order to develop passive mechanical metamaterials with excellent stiffness, strength and lightweight properties.

Specific properties are another set of essential parameters for assessing the performance of passive mechanical metamaterials. They are defined as $\left(\frac{E^*}{\rho^*}\right)$ and $\left(\frac{\sigma^*}{\rho^*}\right)$ for specific stiffness and specific strength, respectively, and enable comparison of topological arrangements with different apparent densities. Multiple research publications emphasise the importance of using specific properties to adequately compare lightweight materials and structures [4, 75, 79] and therefore they are used extensively throughout the chapters of this thesis.
2.1. MECHANICAL METAMATERIALS

Utilising the concepts presented here, the following sections categorise 3D phase topologies used in passive mechanical metamaterials according to their geometrical features: lattices, thin-walled structures and minimal surface-based topologies are discussed. The following sections further emphasise the benefits of stretch-dominated structures over bending-dominated ones, compare their specific properties and present the most relevant research publications.

2.1.2 Lattice structures

Lattice structures are among the most broadly used mechanical metamaterial topologies [75]. They are made of strut elements, commonly, of the same radius and length, for example, circular cross-section rods, which connect together at shared joints. The mechanical performance and stretch or bending-dominated behaviour of these structures are dictated by the nodal connectivity at the joints. The rigidity is described using Maxwell’s stability criterion \( M \) which are shown in Equation 2.1 and Equation 2.2 for 2D and 3D lattices, respectively:

\[
M = b - 2j + 3 \quad (2.1)
\]

\[
M = b - 3j + 6 \quad (2.2)
\]

where, \( b \) is the number of struts and \( j \) is the number of frictionless joints. For the structure to be stretch-dominated, the necessary condition for rigidity is met when \( M = 0 \) and all the members carry a load in either tension or compression. When this condition is satisfied, introducing stiff rather than frictionless joints does not make a difference as slender elements of the structure are much stiffer when stretched rather than bent [7]. If \( M < 0 \), the structure does not maintain the rigidity and deforms as a mechanism while in the case of \( M > 0 \), the structure is overconstrained and is likely to behave as a bending-dominated structure. Examining the presented equations also reveals that random topological arrangements, such as the ones found in foams, tend to be overconstrained and hence, behave in a bending-dominated manner [80]. Nevertheless, the Maxwell rule has its limitations and only applies to lattice structures with low apparent densities. If the elements are thicker (i.e. stockier) and cannot be considered slender, the geometry of the joints needs to be taken into account and
therefore, the relationship previously described using the power scaling law no longer applies [80].

A few stretch-dominated lattice examples include, but are not limited to, isotropic trusses [5, 81], several variations of cube-like structures [6, 82] such as face-diagonal [82], body-centred [82, 83, 84] and truncated cube [83, 85]. Additionally, multiple publications investigate the performance of octahedron [82, 86], void octet [82] and the combination of the two which is the octet truss [2, 87, 88, 89]. The octet truss is one of the most commonly studied lattice structures in the literature having high stiffness and load-bearing capacity as demonstrated by [87] and can be optimised to develop ultra-stiff and light metamaterials [2, 76]. The octet truss structure is a fully triangulated structure with its truss members deforming axially when loaded and therefore well illustrating the benefits of stretch-dominated structures. However, the structure is less suitable for mixed-mode loading conditions as the slender members of the octet truss tend to fail in buckling [87]. Figure 2.2 shows some of the stretch-dominated lattice structures in blue and also a few bending-dominated ones in green. A few examples of the latter type include ideal open-cell foam [7], truncated octahedron [6] and Kelvin lattice [8].

Figure 2.2: Examples of stretch-dominated (in blue) and bending-dominated (in green) 3D structures. The representations are adapted from [5, 6, 7, 8].
2.1.3 Thin-walled structures

Thin-walled structures refer to a type of mechanical metamaterials made of thin angled plate-like features connected at their edges, usually forming closed unit cell structures in 3D (see Figure 2.3). This arrangement was shown to reduce configurational entropy within the structure. Hence, it increases strain energy storage capacity and also provides multi-axial stiffness higher than lattice structures where each beam only supports axial forces [90, 91]. Under the applied load, the individual thin-walled features develop membrane stresses along multiple in-plane directions leading to stretch-dominated behaviour [75], the benefits of which were discussed in Section 2.1.1. Due to such topological configuration advantage, Young’s modulus of an optimal thin-walled structure can be up to three times greater in comparison to an optimal lattice-based topology [92]. This was also shown using numerical simulations by Berger et al. [5] in 2017 who compared an octet truss with an octet foam structure, where the latter was shown to be almost three times stiffer than the former. In fact, the same study demonstrated that an optimised “cubic + octet” topology as shown in Figure 2.3 can achieve the theoretical upper bound for stiffness and strain energy storage. In 2020, a publication by Wang et al. [9] also showed that the theoretical upper stiffness bound, also known as Hashin–Shtrikman (H–S) upper bound of elastic stiffness, can be achieved by using low density (i.e. thin wall) n-fold symmetric thin-walled cells. A few other examples of 3D stretch-dominated structures include but are not limited to thin-walled closed cells based on cubic [10], octet [5, 10] and tetrakaidecahedron [11] geometries. All of the mentioned 3D unit cell structures discussed in this section are illustrated in the top half of Figure 2.3.

Although 3D thin-walled closed-cell structures show higher stiffness properties in comparison to other types of geometries employed for metamaterial development, they suffer from manufacturability issues when certain additive manufacturing (AM) processes are used. Three out of the seven AM methods classified by the International Organization for Standardization (ISO) and American Society for Testing and Materials (ASTM) 52900:2015 standard [93] are not suitable for manufacturing closed-cell cellular solids due to the inability to clear printing material trapped inside the closed unit cells [94]. These three methods are namely, binder jetting (BJ), powder bed fusion (PBF) and var photopolymerization (VP). The first two are powder-bed-based processes leaving powder trapped in the closed cavities while the third method uses a liquid-bath approach leaving residual resin trapped inside the closed unit cells. In the
2.1. MECHANICAL METAMATERIALS

Figure 2.3: Examples of stretch-dominated thin-walled geometries in 3D (in red) and in 2D (in yellow). The representations are adapted from [5, 9, 10, 11].

published literature, this limitation is sometimes referred to as the main roadblock for the adoption of thin-walled mechanical metamaterial [94] and is addressed by introducing geometrical features, most commonly circular holes, that allow for powder removal or resin drainage. The work presented by Tancogne-Dejean et al. [94] demonstrates that an optimal design of these drainage or powder removal features negatively affects the overall stiffness of the thin-walled structure by as little as 5%.

The significance of these findings is evident considering that the powder bed fusion (PBF) and var photopolymerization (VP), together with the material extrusion (ME) method, otherwise known as fused deposition modelling (FDM), are among the most affordable approaches in additive manufacturing [95, 96]. This limitation of 3D thin-walled closed-cell structures also applies to 4-polytope-based metamaterials, further discussed in Section 2.2 of this chapter. The employed mitigation techniques in this thesis are similar to the solutions presented in the literature and are discussed in detail in Chapter 3.

2D honeycomb structures of various shapes, including but not limited to hexagonal [46, 97], square [98, 99] and diamond arrangements [98, 100], are also in the 2D thin-walled structure category. They are shown in the lower half of Figure 2.3.

The open-cell geometries, with plate-like features oriented in a direction perpendicular to one of the orthogonal axes, share similar advantages with the 3D closed-cell
topologies in restraining the number of deformation modes and therefore, increasing elastic energy storage capacity [75]. However, due to the 2D nature, the mechanical performance of these structures varies significantly when comparing in-plane and out-of-plane loading directions. Nevertheless, 2D honeycombs offer a low cost-to-benefit ratio [90] and are commonly used for applications requiring high specific stiffness. Due to this reason, hexagonal honeycomb structures closely mimicking a honeycomb core (CEL Components - PP8.120T30 industry product) [101] are employed throughout this thesis as one of the benchmarking geometries aiding in comparing 4-polytope-based structures with commercially available lightweight products.

2.1.4 Minimal surface structures

Minimal surface structures are another category of passive mechanical metamaterials associated with stiffness and lightweightness. They are similar to thin-walled structures, discussed in Section 2.1.3, as they are made of thin, continuous shells, however, these shells have a curvature. Mathematically, minimal surface geometries are defined as surfaces with the mean curvatures (the average value of the principal curvatures - \((\kappa_1 + \kappa_2)/2\), where \(\kappa\) represents the curvature of a curve) being equal to zero while their Gaussian curvatures (the product of the principal curvatures - \(\kappa_1\kappa_2\)) have a negative value at any point on this curved geometry [102]. A more intuitive explanation can be formulated by analysing physical models representing minimal surfaces. When a wireframe is dipped into a soap solution, a thin film forms across the edges of the shape. Due to the surface tension, the film arranges itself to minimise the total area of the surface hence creating a minimal surface. Research in [103] has shown that when this concept is applied to mechanical metamaterials and the structure is loaded, the minimal surface shells experience in-plane straining which leads to stretch-dominated behaviour, the benefits of which were previously described in Section 2.1.1. Additionally, the presence of smooth curves and lack of nodal joints or sharp edges connecting thin plates, unlike in lattice and thin-walled structures, reduces the number of stress concentration points leading to premature local failure within the structure [104, 105].

In the field of mechanical metamaterials, the term triply periodic minimal surfaces (TPMS) is often used to describe shellular structures, a category of cellular structures also referred to as shell cellular, with the unit cell repeated in 3-dimensions. The reviewed literature revealed that Neovius [13, 106], IWP [12], P [12, 17] and D [107]
2.1. MECHANICAL METAMATERIALS

Shellular and gyroid (G shellular) [3, 107] surfaces are among a few examples of stretch-dominated topologies in this category (shown in Figure 2.4). A publication by Nguyen et al. [12] demonstrated that P shellular geometries can achieve superior strength in comparison to ultra-low density lattices ($\rho_s/\rho_s \approx 0.01$). For this reason, the aforementioned structure serves as a benchmark against which newly proposed 4-polytope-based metamaterials are compared in Chapter 5.

![Examples of triply periodic minimal surface structures.](image)

Figure 2.4: Examples of triply periodic minimal surface structures. The representations are adapted from [12, 13].

Nevertheless, one of the most significant publications on minimal surface metamaterials is by Qin et al. [3] investigating the mechanical strength of optimal gyroid (G shellular) structures. The findings presented in this study claim that the gyroid topological arrangement represents an idealised atomic 3D graphene structure which if manufactured using graphene flakes could potentially achieve 10 times the tensile strength of mild steel while having a density as low as 4.6% of mild steel. These results were obtained using molecular dynamics simulations to evaluate internal interactions of carbon atoms within the 3D graphene assembly. The researchers attribute such a superior performance to both the graphene properties and the topological arrangement of the structure. Due to the latter reason, the gyroid is chosen as another benchmarking unit cell geometry used in this work. Chapters 4, 5 and 6 investigate the performance of 4-polytope-based metamaterials in compression, tension and shear, along with the gyroid and hexagonal honeycomb structures, previously discussed in Section 2.1.3, and compare their mechanical behaviour against each other. Using the same manufacturing methodology (later discussed in Chapter 3) for all of the mentioned geometries, minimises the effects of material and manufacturing-related discrepancies between the samples and allows for a direct comparison of the analysed structures.
2.1. MECHANICAL METAMATERIALS

2.1.5 Shear stiff structures

While the majority of research to date concerns the axial loading of mechanical metamaterials, there have been far fewer efforts that have considered shear loading and the development of shear stiff structures. Yet, shear loading is ubiquitous in engineered structures and an aim should be to more commonly factor shear into the design process of novel passive mechanical metamaterials. Among the papers that have considered shear stiff structures, several publications present findings on 3D lattices [4, 108, 109, 110]. Octet truss, previously discussed in Section 2.1.2, is one of the most commonly employed topologies for developing shear stiff metamaterials. Dong et al. [110] demonstrated that the octet topology is able to outperform polymer and metal foams in terms of shear modulus and shear strength properties. Other examples of lattice-like structures are mostly limited to geometrically simple lattice types such as tetrahedral [108] and prismatic-type trusses [109].

Another research trend in the published literature is to use 2D thin-walled structures, previously discussed in Section 2.1.3. Various 2D honeycomb geometries, such as hexagonal [97], square [99] and diamond honeycombs [100], are most commonly used and their most prevailing application is in developing sandwich panels. Work presented by Jiménez et al. [111] demonstrates the superiority of square and hexagonal honeycombs for producing high shear stiffness-to-weight ratio structures in comparison to other 2D thin-walled cellular structures.

The widespread use of 2D honeycombs is attributed to their cost effectiveness [90] even though 2D thin-walled structures are not inherently shear stiff, with high out-of-plane but low in-plane stiffness. This suggests that 3D thin-walled structures offering stiffness along all three orthogonal directions should be more suitable for similar applications. Nevertheless, there is an evident research gap in this area as shown by the most recent reviews published in the field [4, 75]. Addressing this gap, part of this thesis, specifically Chapter 6, considers the use of 4-polytope-based structures as the building blocks for shear stiff metamaterials.

In the following section of this literature review, the theory behind 4-polytope concepts, their representation in 3D space and their potential geometrical benefits are discussed in more detail. The section provides a more detailed description of how the 4D geometries can be used to design stiff, strong and lightweight mechanical metamaterials.
The concept of 4-polytopes and their potential suitability for mechanical applications due to their symmetrical and self-repeating features was introduced in Section 1.4 of Chapter 1. As it is evident from the literature reviewed in Section 2.1 of this chapter, the concept of 4-polytopes, to the best of our knowledge, has never been applied in the context of designing passive mechanical metamaterials for stiffness, strength and lightweightness. This section summarises the geometrical theory relevant to the 4-polytopes used in this work and provides the justification for choosing the regular convex 4-polytopes as the basis for mechanical metamaterial development.

2.2.1 Regular and convex polytopes

In geometric theory, regularity is defined by assessing the degree of polytope symmetry. In 2D space, a polygon (2-polytope) is regular if all of its edges and interior angles are equal [112]. Additionally, a polygon is also convex when all of its sides are pointing outward or, in other words, when each of the internal angles is less than 180° [113]. To give a few examples, an equilateral triangle is a regular convex polygon with three sides ($p = 3$) and so is a square with four sides ($p = 4$), a pentagon with five ($p = 5$) and so on. In fact, there is an infinite number of regular 2-polytopes as $p \to \infty$. The number of sides ($p$), in the case of 2-polytopes, is also a Schlafli symbol, \{p\}, of a polygon.

In 3D space, there are five regular convex polyhedra (3-polytopes) which have the same number of identical faces that meet at each vertex. They are referred to as the five platonic solids, namely the tetrahedron, cube, octahedron, dodecahedron and icosahedron [112]. Each one of these is built by putting regular polygons around a shared vertex on a 2D plane and folding the pattern into the 3rd dimension. In this manner, a 3-polytope such as a cube is formed using two sets of three squares (Figure 2.5 (a)) which are “pushed” into the 3D space around the same vertex (Figure 2.5 (b)) by folding this pattern. The newly formed polyhedron is, therefore, a regular convex 3-polytope (Figure 2.5 (c)) assembled from regular convex 2-polytopes. In this case, the Schlafli symbol of a cube is \{4,3\}, following \{p,q\} representation for 3-polytopes, as it is made of squares ($p = 4$) and has three ($q = 3$) of them around each vertex.
2.2. 4-POLYTOPE-BASED STRUCTURES: A NEW CLASS OF MECHANICAL METAMATERIALS

The same principles apply to forming 4-polytopes. In the case of a tesseract (hypercube), three cubes are arranged around an edge and “pushed” into the 4D space to create parts of this 4-polytope, which when assembled is made of 8 cubes in total. Hence, the tesseract is also often referred to as the 8-cell. The Schlafli symbol of this newly formed 4-polytope is then \{4, 3, 3\}, following \{p, q, r\} representation for 4-polytopes, as it is made of cubes, \{4, 3\}, and has three (r = 3) of them around each edge. Following the same convention, all regular convex 4-polytopes and their Schlafli symbols are listed in Table 2.1.

Table 2.1: Regular convex 4-polytopes and their respective Schlafli symbols.

<table>
<thead>
<tr>
<th>Names:</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>120-cell</th>
<th>600-cell</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pentamode</td>
<td>Tesseract</td>
<td>Orthoplex</td>
<td>Octaplex</td>
<td>Dodecaplex</td>
<td>Tetraplex</td>
</tr>
<tr>
<td>Schlafli symbol:</td>
<td>{3, 3, 3}</td>
<td>{4, 3, 3}</td>
<td>{3, 3, 4}</td>
<td>{3, 4, 3}</td>
<td>{5, 3, 3}</td>
<td>{3, 3, 5}</td>
</tr>
</tbody>
</table>

2.2.2 Schlegel diagram

Although 4-polytopes can be described using Schlafli symbols, they cannot ordinarily be visualised or rendered in 3D. Therefore, they are often represented as 3D wire-frames of 4-polytopes. Projecting a geometry from \(\mathbb{R}^n\) space to a lower dimension
2.2. 4-POLYTOPE-BASED STRUCTURES: A NEW CLASS OF MECHANICAL METAMATERIALS

$\mathbb{R}^{n-1}$ space, allows us to visualise 4-polytopes without using time as a substitute for the 4th dimension and therefore render these objects as static structures [114].

![Figure 2.6: A diagram illustrating a projection of a cube (a 3D geometry) to 2D space. The formed image in blue is a Schlegel diagram of a cube.](image)

This concept, in principle, is the same as projecting a cube into a 2D space. Depending on the projection type and angle, an infinite range of 2D geometries can be created from a single 3D object. To circumvent this problem and to limit the number of resulting structures to one, the 4-polytopes further investigated in this work are only represented using Schlegel diagrams. Employing this method allows to construct a projection using a point just outside one of the polytope facets. The location of this point (centre of projection) is chosen so that it is close to the middle of the mentioned facet as represented by the blue dot in Figure 2.6 showing a Schlegel diagram of a cube being projected to a 2D plane. Therefore, the created projection of this facet completely contains the projections of all the remaining facets of the polytope. This results in a diagram where (1) the facet closest to the centre of the projection appears the largest, (2) the edges that were parallel to the facet remain parallel to it in the diagram and (3) the edges that were perpendicular to the facet converge to a point [114].

Using the method described for the polytopes of lower dimensions, Figure 2.7 shows the constructed Schlegel diagrams of all six regular convex 4-polytopes. Due to the location of the centre of projection, the wireframe structures maintain the high regularity of the regular convex 4-polytopes when rendered in 3D space.
2.2. 4-POLYTOPE-BASED STRUCTURES: A NEW CLASS OF MECHANICAL METAMATERIALS

Figure 2.7: Examples of regular 4-polytopes shown as 3D wireframes. The dashed line identifies the four wireframes further analysed in this thesis.

2.2.3 4-polytope applications in mechanical metamaterials

Figure 2.7 also illustrates the geometrical complexity of each 4-polytope when projected to the 3D space. As the number of cells in each 4-polytope increases, the internal wireframe features become progressively smaller with respect to the rest of the structure. This becomes a key consideration when the wireframe structures are scaled to create a single metamaterial unit cell which has external dimensions in the range of 10-15mm, (further discussed in Section 3.1.1 of Chapter 3). Hence, the internal wireframe features of the more complex 4-polytope, namely 120-cell and 600-cell, become too small to be accurately manufactured as their geometrical size at this scale is close to the accuracy of the manufacturing methods used to produce metamaterial samples (Section 3.4 of Chapter 3). Due to this reason, only four out of the six wireframes illustrated in this figure, namely the 5-cell, 8-cell, 16-cell and 24-cell, are further investigated in this work and used as the basis for mechanical metamaterial unit cell designs. As these structures are derived from regular convex polytopes using Schlegel diagrams they maintain a highly symmetrical nature [114]. This is considered of high importance for the application of these wireframes in mechanical
Employing a range of 4-polytopes wireframe structures as the basis for mechanical metamaterial development is novel and has not been published in the literature. As shown in the previous sections of this chapter, 3D projected 4-polytopes have geometrical features which are self-repeating and hierarchical, benefiting from multiple symmetry planes within the polytope, and as such, are expected to show great potential in applications where high global stiffness and lightweightness are required [55, 115, 116]. However, there is a research gap in exploring these structures for mechanical applications.

While the 4-polytopes are well understood in mathematics, in general, their application is limited to a few niche fields. Due to their geometrical symmetry and self-repeating features when projected as 3D structures, 4-polytopes have been of interest in aesthetic design and can be seen in some patterned materials, ornaments and creative sculptures [56, 57, 58]. Another example is in the field of computer modelling with several reports on the more technical utility of 4-polytopes, for example, as space-discretising finite elements [117, 118, 119, 120]. To the best of our knowledge, there are only two other publications related to investigating the tesseract (8-cell) wireframe structures in the context of mechanical or structural design applications. One of them considers a tesseract projection as an additively manufactured high-porosity potential bone replacement material [121] while the second one [122] discusses the strength and stiffness of strut-based tesseract wireframes. Both of the publications focus only on the tesseract structure in a limited capacity without investigating other 4-polytope-based structures.

This demonstrates that there is an obvious gap in knowledge concerning the development of 4-polytope-based mechanical metamaterials, which this thesis aims to address. The work presented herein considers the suitability of 3D projected 4-polytopes as base structures for the development of novel mechanical metamaterials.

The surveyed literature presented thus far emphasised the importance of selecting a suitable topology when designing stiff, strong and lightweight mechanical metamaterials. Some of the studies indicated that the top-performing structures were developed by choosing the optimal or optimised topological arrangement, however, the concepts of optimisation have not been discussed so far. Therefore, the following section reviews the optimisation and computational design approaches employed
in the field of metamaterial design and presents the most commonly used problem-specific approaches.

2.3 Optimisation and computational design

This section of the literature review discusses the use of algorithms employed in the optimisation and computational design of mechanical metamaterials. First, it discusses the different algorithm types, identifies their application areas and describes the importance of parametric optimisation for mechanical metamaterial design. Then, it analyses the different methods employed in the literature to implement parametric optimisation and reviews their suitability for the development of 4-polytope-based metamaterials.

2.3.1 AI and nature-inspired optimisation algorithms

In this work, over 280 peer-reviewed publications were surveyed to investigate the use of AI and optimisation techniques most commonly employed in designing metamaterials or enhancing their performance. As the current metamaterial development process heavily relies on modelling and simulation outcomes, the integration of these techniques not only enables the exploration of a larger design space but also allows for partial or even complete automation of the design process. It should be noted that in this chapter, only the analysis and literature relevant to the scope and methodology of this thesis are included. The complete analysis will be published as a standalone output.

Through this extensive review, the most popular techniques, by the number of publications, were found to be evolutionary algorithms and artificial neural networks (ANN). In fact, around half of the reviewed publications adopt evolutionary algorithms in some capacity with neural networks being the second most frequently utilised method and less than 10% of the reviewed publications applying other AI approaches such as gradient-based methods [123], dimensionality reduction techniques [124, 125] and Bayesian optimisation or machine learning methods [126, 127, 128].

This trend is illustrated in Figure 2.8 where the reviewed publications are split according to their main AI and optimisation techniques, namely, (1) artificial neural
2.3. **OPTIMISATION AND COMPUTATIONAL DESIGN**

Figure 2.8: Increasing trend of different AI-based and nature-inspired techniques in mechanical metamaterial design.

networks (ANN), (2) nature-inspired optimization techniques, such as genetic algorithm (GA) and swarm intelligence, and (3) ML algorithms, a cluster of techniques other than nature-inspired and ANN approaches. Although this categorisation, with all of the remaining approaches being included in the third category, is limiting in terms of discussing the full range of available AI and optimisation methods, the purpose of it is to illustrate the most commonly used methods in mechanical metamaterial design, in particular, the approaches relevant to the work presented in this thesis.

Figure 2.8 also indicates that the use of computational design and optimisation approaches in metamaterial design is growing. Over the past decade, nature-inspired algorithms have been the most widely utilised method, however, ANNs are becoming more popular and are unlocking new design and optimisation capabilities. The surveyed literature also showed that the dominant application areas of ANNs and nature-inspired algorithms differ and that these techniques are not direct substitutes for one another. Whilst ANN approaches are used for mainly four specific applications namely, inverse design, surrogate modelling, classification and clustering and generating new material structures based on the knowledge captured in the training data, nature-inspired algorithms have a narrower but well-defined range of differing applications. They are mostly used for two optimisation purposes which are metamaterial structure parameter optimisation and optimisation for inverse design purposes.

It should be noted that as this thesis performs parametric optimisation of 4-polytope-based structures, later described in Chapter 3, only this application of AI
and optimisation techniques is discussed further in this chapter. The following section describes the nature of the parametric design problem and presents the most commonly employed nature-inspired algorithms to perform parametric optimisation of metamaterial structures.

### 2.3.2 Parametric optimisation of mechanical metamaterials

Parametric optimisation refers to the process of finding the most suitable arrangement of the given parameters that result in maximising or minimising a defined objective function [129]. In the context of mechanical metamaterials, the objective is mostly formulated to enhance a certain property such as maximising the stiffness and strength of a structure or minimising its mass. The optimisation problem is usually formulated to suit a specific application considering given loading and boundary conditions. A few examples may include optimising the topological arrangement of a metamaterial to enhance tensile properties [130], selecting the most suitable bulk materials from a database to ensure material compatibility [131] or arranging metamaterial building blocks to form a metamaterial array [132].

The surveyed literature has shown that parametric optimisation problems in the mechanical metamaterial design field are almost solely solved using nature-inspired algorithms. These algorithms are meta-heuristic approaches inspired by genetic evolution or swarm intelligence. They are designed to have a stochastic search behaviour and iteratively explore the design space by using intelligent search strategies [133]. This is highly advantageous for solving optimisation problems where using conventional methods may be insufficient or not feasible due to the complexity of the problem, large search space or non-linearity of the objective function [133, 134]. The success of this category of algorithms is attributed to their simplicity, flexibility, high adaptability and efficiency [129, 135]. Additionally, they are easy to implement using most programming languages and can be easily incorporated into the existing metamaterial design frameworks [129]. Nevertheless, meta-heuristic optimisation algorithms are often considered to be more computationally expensive than other techniques. They tend to find sub-optimal solutions which are close but not exactly at the global maxima (or global minima) and they do not scale well with the increasing complexity of a problem [136, 137].

The following sections of this literature review the two most commonly employed nature-inspired optimisation algorithms used in mechanical metamaterial design. In
2.3. OPTIMISATION AND COMPUTATIONAL DESIGN

In particular, various GA types and particle swarm intelligence methods are discussed in Sections 2.3.2.1 and 2.3.2.2 respectively while Section 2.3.2.3 presents the reasoning for choosing GA as the most suitable for the parametric optimisation of 4-polytope-based metamaterials.

2.3.2.1 Genetic algorithm

In the published literature on mechanical metamaterial design, various types of GA are commonly employed in solving parametric optimisation problems. They are also sometimes referred to as evolutionary algorithms and as the name suggests, they use genetic operators such as reproduction, mutation, recombination and selection to evolve the population and advance towards a solution. GA is a highly exploratory approach as each individual within the generation acts as an independent agent looking for the most optimum solution with the computations being executed in parallel [133, 138]. One of the strengths of these algorithms is the fact that no gradient information is needed to perform optimisation. Due to this reason, GA is the most prevailing method for solving parametric optimisation problems within the mechanical metamaterial design field [135] where design inputs cannot be directly correlated to the outputs or, in other words, the behaviour of a metamaterial structure. A more in-depth description of the algorithm is provided in Section 3.3 of Chapter 3 along with the schematic representation of the design process in Figure 3.9.

GA is often used for metamaterial development processes that heavily rely on finite element analysis or other computationally expensive metamaterial performance evaluation techniques. A publication by Qiu et al. [139] demonstrates a GA-powered optimisation framework that iterates the parameters within the design domain and then evaluates the resulting metamaterial structures using finite element analysis (FEA). A similar optimisation approach is demonstrated in [140] when a single objective GA is used to enhance the performance of auxetic structures. Multiple other studies have shown the benefits of combining FEA and GA-based optimisation to develop lattice structures [139, 141], auxetic structures [63, 140, 142] and cellular solids [143, 144]. Due to the versatility of these algorithms, this approach can be coupled with analysis methods other than numerical simulations. Wang et al. [145] present a parametric optimisation of honeycomb structures where the metamaterial response is analysed using analytical Castigliano’s theorem with the objective to enhance auxetic proper-
ties while respecting the mass constraints. This robustness and versatility of GAs is highly suited for a wide range of parametric optimisation problems [129, 135].

A number of research publications also demonstrate the use of GAs in multi-objective optimisation. Cimolai et al. [130] demonstrates a single-population GA finding a solution to an objective function with two conflicting objectives. The algorithm minimises the mass while also maximising the tensile range of a metamaterial structure. A publication by Liu et al. [143] presents findings on using a multi-objective micro-GA, a variation with a small population size, to find optimal solutions of periodic and non-periodic metamaterial structures at the same time. Other multi-objective examples most commonly found in literature use a non-dominated sorting GA (NSGA) to sort possible optimum solutions into Pareto fronts and allow the designer to choose the best-suited metamaterial design satisfying both of the conflicting objectives [42, 141, 144]. A few examples include optimising for variable stiffness while minimising the maximum stress [42], maintaining isotropic properties while increasing auxetic properties [141] and reducing initial peak crushing force without sacrificing overall energy absorption [144].

Multi-island GA is often seen in the literature for optimisation problems that would otherwise converge to a local minima using a single-population GA configuration [129, 135]. The work presented in [145] shows that choosing a multi-island GA configuration for a specific parametric optimisation problem in auxetic structures allowed them to explore the full parameter range and avoid locally optimum solutions. Wang et al. [142] also demonstrated the use of multi-island GA in designing cut-mediated soft mechanical metamaterials emphasising the advantages of this GA type.

### 2.3.2.2 Particle swarm intelligence

In addition to GA, particle swarm optimisation (PSO) is also used as a nature-inspired meta-heuristic algorithm to achieve optimisation in mechanical metamaterial design. This algorithm mimics the search behaviour of an intelligent biological swarm to arrive at the optimal solution. A study published by Singleton et al. [146] showed that the PSO algorithm finds a solution quicker in comparison to GAs, however, suffers from local minima convergence issues, which were previously discussed in Section 2.3.2.1. In the context of mechanical metamaterial design, only a few publications using PSO were found. The algorithm was shown to be suitable for finding the optimum folding
patterns (origami-based patterns) when assembling metamaterial mechanisms [147] and producing metamaterial structures from flat and foldable sheets [148]. Nevertheless, none of the aforementioned studies focus on optimising the topological arrangement of mechanical metamaterial structures and therefore are not found relevant to the work presented in this thesis.

2.3.2.3 Justification for the algorithm choice in this work

To summarise, the surveyed literature shows that GAs are most commonly employed for the parametric optimisation of mechanical metamaterials. In fact, various types of GAs are almost solely used for the discussed optimisation problem. The single-objective GA was shown to perform well across a variety of optimisation tasks involving the development of lattice structures [139, 141], auxetic structures [63, 140, 142] and cellular solids [143, 144]. Several publications present the use of more complex, advanced variations of GA, such as micro-population, multi-island, multi-objective GA or particle swarm intelligence-based approaches. These algorithms were shown to be more suited for specific design tasks when the search space was well understood or when a single-population GA yielded convergence to local rather than global minima. The parametric optimisation carried out in this work, further described in Section 3.3 of Chapter 3, is based on a single-population GA which is found to be the most suitable for a single-objective problem formulated for this metamaterial design task.

2.4 Industrial use of mechanical metamaterials

As mechanical materials research is still not widely adopted in industrial applications, the research to date has focused on the demonstration and validation of their performance due to the architected features. Nevertheless, mechanical metamaterials have not yet been widely adopted in engineering sectors such as automotive, aviation and energy which are pursuing lightweight solutions. The key reason for this is the issue of scaling up additive manufacturing, although some research is being carried out to circumvent this limitation [96, 149, 150].

In this section, three examples are presented which demonstrate the use of mechanical metamaterials for three distinctly different industrial uses. As shown in Figure 2.9, these are (a) meta-implants (hip stem replacements) in bio-engineering [14], (b)
2.4. INDUSTRIAL USE OF MECHANICAL METAMATERIALS

Figure 2.9: Three examples of industry applications which include (a) meta-implants (hip stems) [14], (b) morphing airfoils [15] and (c) high-end athletic footwear [16].

morphing airfoils [15] in the aerospace industry and (c) high-end athletic footwear designed collaboratively by Carbon and Adidas [16].

As presented previously, there are several proposed application areas for mechanical metamaterials, however, only a few have led to real product development and commercial use. Examples [16] and [151] demonstrate the utilisation of 3D printing in the athletic footwear market with architected midsole trainers for high-end customised products.

Mechanical metamaterials have also found their application in the biomedical field where they are often referred to as “meta-biomaterials”. Kolken et al. [14] designed hip stems using a metamaterials approach which are hence called “meta-implants”. This was performed such that compression is applied on both sides of the part, made of structures with negative and positive Poisson’s ratios. As a result, this novel meta-implant design was shown to improve implant-to-bone contact when it is used in an artificial hip replacement surgery. Additionally, there are proposed studies on the use of metamaterials for stent and skin graft applications such as the work in [152] which used hierarchical multi-level rotating squares to develop auxetic structures. Lastly, 3D nano-scale metamaterials were proposed by Maggi et al. [153] to achieve more efficient bone tissue growth. Using UV radiation, the stiffness of the bio-compatible
polymer, namely OrmoCorp, was adjusted to match the stiffness of bone cartilage which had a positive effect on the cell growth rate.

Given the properties of mechanical metamaterials, they are also suitable for use in the aerospace industry [154]. Bettini et al. [15] demonstrated the adoption of composite metamaterials in morphing aerofoils. The developed structure was shown to have the ability of sustaining large deformations while experiencing smaller local material strains in comparison to the conventional solutions under the same loading conditions. Further development of lightweight functional mechanical metamaterials is expected to accelerate their adoption for morphing components in the aerospace and renewable energy sectors.

2.5 Summary and key recommendations

To summarise, this chapter presented the relevant previous work which formed the foundation of this thesis. Firstly, four types of mechanical materials, including lattice, thin-walled, minimal surface and shear stiff structures, were reviewed in Section 2.1. Secondly, in Section 2.2, the theory of 4-polytopes was explained building upon the principles which are well known in mathematics and geometry. Nevertheless, these concepts have not yet been adopted for engineering applications which is one of the novelties of this work. This section also introduced the 4D to 3D projection of 4-polytopes which is taken further as the basis for metamaterial unit cell design in Section 3.1 of Chapter 3. Thirdly, the mechanical metamaterial literature was surveyed to analyse the use of AI and optimisation. This was later narrowed down to fit the scope of this thesis which focuses on parametric optimisation. As shown in Section 2.3, the most prominent and suitable method was identified as GA which is later described in detail in Section 3.3 of Chapter 3. Lastly, a wider outlook was adopted to showcase the use of mechanical metamaterials in industry. This discussion is taken further in Chapter 7. In particular, Section 7.4 reviews the emerging applications and foreseen challenges for the future development of mechanical metamaterials.

Following the literature review, key recommendations are presented below for future research:

- For wider adoption of mechanical metamaterials in industry, standardised testing and benchmarking against widely adopted and best performing structures are needed. This work uses (1) a commercially available honeycomb structure
and (2) a 3D gyroid to initiate this standardised method of comparison in the field.

- While 4-polytopes are well-known in the field of mathematics and geometry, their potential in metamaterial design has not yet been explored. This is one of the key novelties of this work, however, this area still remains underresearched.

- As the design of mechanical material includes complex optimisation problems with various interlinked variables, metaheuristic and AI methods have the potential to accelerate the design process. For parametric optimisation, GA was shown to be the most prevailing method and accordingly, it was adopted for use in this thesis. There is a need for better understanding and documentation of AI and optimisation techniques used in this field.

- Lastly, open source data would not only contribute to the knowledge within the research community but would also increase the transparency of the work. Hence, it would help foster collaborations with industry to find suitable uses for mechanical metamaterials in engineering. In line with this recommendation, all results from this work are made available in open-access data repositories listed in Section 1.9 of Chapter 1.
Chapter 3

Methods for designing, optimising, manufacturing and testing 4-polytope-based metamaterials

This chapter introduces the methodology employed in this work which ranges from the design, simulation and optimisation of the 4-polytope-based mechanical materials to their manufacturing and testing. It is divided into five sections where each section focuses on a key methodology: (1) design of metamaterials, (2) unit cell simulations, (3) parametric optimisation, (4) manufacturing and (5) mechanical testing. Parts of this chapter were published in [155, 156, 157].

3.1 Design of 4-polytope-based structures

3.1.1 Unit cell design

Four regular convex 4-polytopes were considered in this work, as baseline geometries for the design of advanced mechanical metamaterial architectures. These are shown in Figure 3.1 as 5-cell (pentatope), 8-cell (tesseract), 16-cell (orthoplex) and 24-cell (octaplex) structures. As shown in this figure, Schlegel diagrams were used to project the 4D geometry as a perspective in 3D space, as previously discussed in Section 2.2.2 of Chapter 2. The method essentially reduces a 4-polytope from 4D to 3D by taking a single projection of the geometry and displaying it as a wireframe in 3D space (3D projected 4-polytope, or, 4-polytope-based structure). Each one of the four wireframe representations of the 4-polytopes shown in Figure 3.1 was used to develop a single metamaterial unit cell by taking the wireframe edges and vertices...
3.1. DESIGN OF 4-POLYTOPE-BASED STRUCTURES

to define the geometry of the thin-walled metamaterials. As the wireframe rendering of the 4-polytopes only provides a geometrical silhouette, the thin-walled features were rendered to match the boundaries of the 4-polytope cell projection as closely as possible. This ensured that the generated thin-walled structures had multiple planes of geometrical symmetry (cubic symmetry of a single cell). From a mechanical perspective, adding geometrical thickness to a wireframe, and hence creating thin-walled features, reduces configurational entropy within the structure which increases the strain energy storage capacity and hence the stiffness of the structure as previously discussed in Section 2.1.3 of Chapter 2. The wireframe structures and their equivalent thin-walled unit cells are shown in Figure 3.1.

![Wireframe Schlegel diagrams](image)

Figure 3.1: Wireframe Schlegel diagrams (perspective projection) of regular convex 4-polytopes (top) and the 4-polytope-based structures designed using the wireframe diagrams (bottom).

The unit cells designed using this approach provide a lot of design flexibility in terms of the structural parameters. As the wireframe representation only illustrates the location of the 4-polytope vertices and edges in the Euclidean space, adding thickness to a wireframe structure allows for the generation of multiple thin-walled metamaterial geometries that originate from the same 4-polytope projection. Additionally, the depth of the perspective can be changed which keeps the same symmetry of the unit cell but results in shrinking or enlarging of the geometrical primitive in the middle of each cell (e.g. the inner cube in the 8-cell). Therefore, by changing
the parameters such as the unit cell wall thickness and the internal geometry angles, the core geometrical shape of the 4-polytope projection is maintained while numerous metamaterial unit cell geometries are generated. As an example, the 5-cell structure was defined using 10 parameters that could be varied to alter the geometrical features in terms of size and shape.

Drain holes were introduced to ensure compatibility with the low force stereolithography (LFS) additive manufacturing (AM) process to allow for a free flow of resin around and inside the thin-walled structures during the printing process. The necessity for the draining features was previously discussed in Section 2.1.3 of Chapter 2, while the choice of LFS additive manufacturing method is justified in Section 3.4 of this chapter. Design parameters for each of the unit cells are shown in Figure 3.2 and these are described in greater detail in Table 3.1. By using this parametric approach to design, the generation of unit cell structures was automated, which took care of any geometrical adjustments necessary in response to loading. The exterior dimensions of a unit cell were not varied as unit cells had to form arrays and these were thus defined by fitting a unit cell into a bounding box cube with a set edge length. This ensured that the unit cells could be manufactured considering the chosen AM limitations and could be stacked in linear arrays to form larger structures comprised of identical repeating unit cells.

![Figure 3.2: Parametric design approach to 4-polytope-based metamaterial design. Adjustable parameters are marked in letters for each structure.](image-url)
### 3.1. DESIGN OF 4-POLYTOPE-BASED STRUCTURES

Table 3.1: Parametric design variables and corresponding descriptions for 5, 8, 16 and 24-cell designs as illustrated in Figure 3.2.

<table>
<thead>
<tr>
<th>5-cell</th>
<th>8-cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>A Drain hole round radius</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>B Drain hole radius</td>
</tr>
<tr>
<td>C Corner distance</td>
<td>C Inner edge round radius</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>D Inner cube size</td>
</tr>
<tr>
<td>E Corner wall thickness</td>
<td>E Outer wall thickness</td>
</tr>
<tr>
<td>F Outer corner round</td>
<td>F Inner cube wall thickness</td>
</tr>
<tr>
<td>G Inner triangle size</td>
<td>G Outer edge round radius</td>
</tr>
<tr>
<td>H Outer shell thickness</td>
<td></td>
</tr>
<tr>
<td>I Outer shell width</td>
<td></td>
</tr>
<tr>
<td>J Outer shell round</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16-cell</th>
<th>24-cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>A Drain hole distance</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>B Drain hole radius</td>
</tr>
<tr>
<td>C Inner triangle size</td>
<td>C Inner triangle size</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>D Inner triangle round</td>
</tr>
<tr>
<td>E Outer shell width</td>
<td>E Projection angle</td>
</tr>
<tr>
<td>F Outer shell round</td>
<td>F Outer shell round</td>
</tr>
<tr>
<td>G Outer shell thickness</td>
<td>G Inner wall thickness</td>
</tr>
<tr>
<td></td>
<td>H Middle wall thickness</td>
</tr>
<tr>
<td></td>
<td>I Outer wall thickness</td>
</tr>
</tbody>
</table>
3.1. DESIGN OF 4-POLYTOPE-BASED STRUCTURES

3.1.2 Stacking of unit cells

The stacking arrangement of the unit cells was chosen to suit each 4-polytope-based geometry. The aim was to maintain the cubic arrangement so that the cubically symmetrical properties of the individual unit cells are transferred to the formed metamaterial array. To achieve this, a stacking pattern with each unit cell having neighbouring cells placed directly on top of each other was chosen. Moreover, the unit cells were arranged in a manner to maximise the contact surface area between the cells and hence the interconnectivity within the array. To address this, the unit cells were mirrored around the outside plane of each unit cell boundary rather than stacked using a linear pattern.

The difference between stacking by mirroring the unit cells and using a linear pattern is illustrated in Figures 3.3 and 3.4. The former presents the case where cells are repeated along the axes (Direction X and Direction Z) to create a metamaterial array. However, it should be noted that due to the geometry of the 5-cell and 16-cell unit cells, which have a diagonal edge at the boundary of each unit cell (marked in red in Figure 3.3), linear stacking arrangement leads to a poor connection between the

![Linear pattern arrangement](image)

Figure 3.3: Schematic representation of a stacking arrangement using the linear pattern where (a) illustrates it along the two axes, which are marked as Direction X and Direction Z, (b) shows the staking along direction X, (c) displays it along both X and Z directions and (d) represents the top view of the resultant metamaterial array.
3.1. DESIGN OF 4-POLYTOPE-BASED STRUCTURES

Figure 3.4: Schematic representation stacking using a mirroring pattern. Where (a) shows the mirroring planes X and Z, (b) displays the mirrored cell across plane X, (c) shows it across both X and Z and (d) represents the top view of the resultant metamaterial array.

neighbouring unit cells. As shown in parts (b) and (c) of the figure, the neighbouring cells are only connected through a small surface area in the middle of the diagonal unit cell edge and therefore such an arrangement is disadvantageous in terms of sharing the load between the neighbouring unit cells. At the boundary between a pair of unit cells, the load is not only concentrated to a small contact area providing a weak interface between the structures but is also causing an onset of bending of the slender diagonal edge elements due to a point load applied. Therefore, if loaded in this arrangement, the corners of the neighbouring unit cells would not share the load and provide overall stiffness to the structure but rather buckle under axially applied loads. The top view of this tiling arrangement is shown in Figure 3.3 (d).

To address this issue, an alternative approach was used which is illustrated in Figure 3.4. The primary unit cell was mirrored across the planes X and Z, to create the neighbouring unit cells. Due to the symmetry of the 4-polytopes, this mirroring arrangement does not create a new geometry (i.e. a mirrored shape of the original cell) but rather produces a shape which is identical to the primary unit cell just rotated by 90°. This effectively creates a connection where the two neighbouring cells
are in full surface contact along their diagonal edges at the boundary. In this case, the interface surface area between the neighbouring unit cells is increased and the transfer of load between the cells does not induce bending of slender edge elements as the corresponding parts of the neighbouring unit cells are acting together to distribute the axial loads. The cross-sectional area at the boundary was designed to be no less than the thinnest cross-section within the individual unit cells connected at that boundary. This ensured that the metamaterial array failure happened within one of the unit cells rather than at the boundary between them. The full set of unit cell parametric design variables is presented in Section 3.1.1.

The aforementioned stacking arrangements only concern the unit cell designs with the diagonal edge elements, namely the 5-cell and the 16-cell. In the case of 8-cell and 24-cell designs, the method of linear pattern and stacking by mirroring the cells results in an identical stacking arrangement as the unit cells are symmetrical across the three orthogonal planes.

Figure 3.5 illustrates the top view of the final stacking arrangement for all four 4-polytope-based mechanical metamaterials. The outcome is a consistent arrangement where the most basic repeating element is shown in colour while the repeating part of the pattern is greyed out. It should be noted that although the 5-cell and 16-cell unit cells do not demonstrate orthogonal symmetry, the shown tiling arrangement, consisting of four unit cells in a 2D plane (8 unit cells in 3D space), becomes the smallest repeatable unit cell pattern which possesses orthogonal symmetry. As these structures also have features of the same length along the three orthogonal axes, the cells are cubically symmetrical. Similarly, due to the inherent cubic symmetry of the 8-cell and 24-cell unit cells themselves, the smallest repeatable pattern in 8-cell and 24-cell cases consists of one unit cell as shown in Figure 3.5.
Figure 3.5: Schematic representation of unit cell stacking approach. The cells shown in colour illustrate the smallest repeated arrangement in each metamaterial case while the shaded areas depict the repetition in the stacking pattern. The markings in red show the interface surfaces between the neighbouring unit cells.
3.2 Unit cell simulations

Finite element analyses were conducted using the Abaqus/Implicit (Dassault Systèmes) solver to determine the properties of each of the 3D projected 4-polytopes subjected to elasto-plastic loading. The mechanical properties of a Formlabs Clear Resin were input into the model as follows: Young’s modulus = 2.03 GPa, Poisson’s ratio = 0.38 and density = 1.164g/cm³. When the model reaches its yield strength, $\sigma_y$, of 72.28 MPa, it undergoes strain softening behaviour over the plastic region of the stress-strain curve, which was approximated using a power regression model as $\sigma_y = 44.99 \times \epsilon_y^{-0.142}$, where $\epsilon_y$ is yield strain. Isotropic hardening was chosen to represent polymer behaviour in the plastic region as all of the investigated loading cases are static. The hardening gradient was governed by the power regression model and was not further adjusted for each of the loading cases. These material parameters were obtained experimentally by testing five cylinder-shaped samples ($n = 5$) in compression, true stress-strain values were used to calibrate the material model. The samples were fabricated using the same additive manufacturing approach later adopted for the metamaterial samples. The manufacturing methodology is further described in Section 3.4 of this chapter.

The Newton-Raphson method was used with an implicit solver as it allowed for variable size increments that were well suited to the simulation problem, providing an accurate solution whilst minimising computational time as compared to an explicit solver. This was recognised by comparing both, the implicit and explicit, solvers. It was found that the implicit solver led to shorter computational times using the simulation set-up and the hardware available. Although the implicit solver tends to have a larger computational cost per single increment when compared to the explicit, it can also benefit from larger increments leading to highly varying increment sizes and therefore, in this case, shorter overall computational times. Therefore, the increment size settings for the static loading problem investigated here were adjusted to be in the range between 0.0001/1 and 1/1 with the initial increment size of 0.01/1. The equation solver settings, solution technique settings and the convergence parameters defining the solution accuracy of nonlinear equations were set to default values within Abaqus/Implicit.

A tetrahedral mesh element (C3D10) was chosen to discretise the structures. Solid rather than shell elements were adopted to allow for the optimisation algorithm to
3.2. UNIT CELL SIMULATIONS

fully explore the design space, i.e., to generate thin as well as thick geometrical elements within the unit cell. A free meshing technique was used as it was found to be the most flexible for meshing when compared to structured and swept meshing approaches. The mesh density was chosen based on mesh convergence studies carried out for each of the 3D projected 4-polytope models, and a mesh growth rate of 1.05 was consequently used to obtain evenly sized elements. Remeshing was introduced by seeding the edges of the geometry. A minimum constraint of three elements across the thinnest feature was implemented and the number of elements increased as the size of any particular geometrical feature increased. This resulted in a mesh density that was fine enough to capture the through-thickness response of the thin-walled features, whilst keeping the number of elements in each model to a minimum.

The mesh convergence study was carried out considering that the models are later used for parametric optimisation of the unit cells during which the initial design geometry is varied and evaluated to find the best-performing design (further discussed in Section 3.3 of this chapter). Therefore, the number of mesh elements was increased incrementally till there was no change in von Mises stress results with the increasing number of mesh elements. The final number of mesh elements in the initial design simulations after performing mesh convergence studies were 84k, 67k, 128k and 123k for the 5, 8, 16 and 24-cell, respectively. This resulted in 139k, 111k, 198k and 200k nodes within each simulation of the 5, 8, 16 and 24-cell. Initial design simulation variable values are listed as “starting values” in Table A.1 within Appendix A. The starting values were set to be the same for all three of the loading cases investigated in this thesis, namely, compression, tension and shear.

During the post-processing stage, the stresses were calculated using the cross-sectional area of the unit cell bounding box and the reaction force outputs at the bottom of the unit cell (location of the encastre boundary condition in each loading case - further discussed in Sections 3.2.1, 3.2.2 and 3.2.3). Similarly, strains were measured considering the height of the bounding box and the displacement at the top of each unit cell (displacement boundary condition). Such an approach yielded stress and strain values for a homogenised metamaterial unit cell and hence provided a reliable method for assessing the performance of a structure regardless of the internal unit cell design.
3.2. UNIT CELL SIMULATIONS

3.2.1 Boundary conditions for the compression set

Boundary conditions were applied to one quarter of each of the 3D projected 4-polytope unit cells, thus taking advantage of the geometrical symmetries to lessen the computational expense. Although the choice of periodic boundary conditions (PBC) is more suited to simulating unit cells in a metamaterial array, symmetric boundary conditions were chosen to reduce computational time without compromising simulation accuracy. This was confirmed by performing separate FE modelling case studies with periodic boundary conditions and with symmetric boundary conditions applied to the models. The comparison of the results showed a difference of less than 0.9% which was considered insignificant when compared to the benefits of reducing computational requirements crucial for the parametric design approach later discussed in Section 3.3 of this chapter. The modelled sections were considered central cells within blocks of neighbouring cells and as such, the outer surfaces of each unit cell were prescribed symmetry boundary conditions about the planes located at the outermost faces of the unit cells, i.e. the interfaces of adjacent unit cells.

Figure 3.6 shows that symmetry boundaries were assigned about the inner X plane (black dashed line) and Z plane (yellow dashed line). The bottom surface of each unit cell was assigned an encastre boundary condition ($U_1 = U_2 = U_3 = UR_1 = UR_2 = UR_3 = 0$), where $U$ is a translation in axes 1, 2 and 3 and $UR$ is a rotation about axes 1, 2 and 3. A displacement condition was assigned to the upper surface of each unit cell. This was chosen over a force constraint to ensure that each unit cell is deformed by the same amount regardless of its internal geometry (generated by the optimisation algorithm) and hence the varying mechanical properties of the unit cell. This approach allowed to obtain absorbed elastic strain energy and reaction force values for each unit cell design and compare them with each other. The displacement value applied at the boundary was chosen so it results in a homogenised unit cell strain of 0.08.

3.2.2 Boundary conditions for the tension set

Similarly to the compression set, all of the 4-polytope-based metamaterials developed for the tensile loading applications can be simulated by exploiting the cubic symmetry of the unit cells. Hence, only one quarter of each unit cell was modelled in order to make the simulations more efficient and reduce the computational time. To achieve
3.2. UNIT CELL SIMULATIONS

Figure 3.6: Boundary conditions of FEA models for 5, 8, 16, 24-cell metamaterial cells (top) and equivalent 4-polytope-based unit cells (bottom). The outer surfaces of a unit cell were prescribed symmetry boundary conditions about the X and Z planes located at the interface between the two adjacent cells. A quarter of each unit cell was modelled by using the internal symmetry planes which are marked in yellow (symmetry about a plane Z) and black (symmetry about a plane X) dashed lines with encastre boundary condition at the bottom and a compressive displacement at the top of the cell.

that, symmetry boundary conditions were prescribed to the inner X plane (orange dashed line) and inner Z plane (red dashed line) as shown in Figure 3.7. To simulate tensile loading conditions, the bottom of each unit cell was set as an encastre boundary condition and the top was prescribed a displacement in the upwards direction. Similarly to modelling the compressive behaviour of the unit cells, case studies comparing the simulations with periodic and with symmetric boundary conditions were carried out and the difference was found to be less than 1.2% between the two cases for the tension set. The displacement value applied at the boundary was chosen so it results in a homogenised unit cell strain of 0.04. To represent the effect of neighbouring unit cells deforming in the same manner, another set of symmetry boundary conditions was used at the outer surfaces (parallel to the X and Z planes) of the quarter unit cells.
3.2. UNIT CELL SIMULATIONS

Figure 3.7: Summary of the boundary conditions applied to 4-polytope-based metamaterial quarter unit cell models (left side) and the full cell illustrations (right side). The outer surfaces of each model were prescribed symmetry boundary conditions about the X and Z planes located at the interface between the neighbouring cells. Orange and red dashed lines on the quarter models (left side) mark the inner X and Z symmetry planes within the unit cells respectively which were prescribed symmetry boundary conditions. An encastre BC was used at the bottom and a tensile displacement BC at the top of each quarter model.

3.2.3 Boundary conditions for the shear set

Unlike the compression and tension cases, full unit cell geometries were simulated for each 4-polytope-based structure to capture the response to shear loading conditions. Encastre boundary condition was applied to the bottom of each unit cell, while a displacement in the direction parallel to the outermost surface was applied at the top of the unit cell. The displacement value applied at the boundary was chosen so it results in a homogenised unit cell shear strain of 0.10. As shown in Figure 3.8, periodic boundary conditions, marked in dark blue, were applied to the outermost surfaces perpendicular to the z-axis. Periodic boundary conditions captured the forces and deformation that an adjacent unit cell could impose on the simulated unit cell. Symmetric instead of periodic boundary conditions were implemented on the surfaces marked in yellow dashed lines as applying them to the surfaces parallel to the shear loading direction (1) did not alter simulation outputs and (2) reduced computational time. The prior statement was confirmed by carrying out separate case studies,
using FEA, with periodic and with symmetric boundary conditions applied to the models. The comparison of the results showed a difference of less than 2% which was considered insignificant taking into account the increase in computational time when simulating the full set of periodic boundary conditions. This is a limitation of the chosen modelling approach which was necessary to carry out parametric optimisation work later discussed in Section 3.3 of this chapter. The set of boundary conditions shown in Figure 3.8 is representative of a unit cell located inside a metamaterial array surrounded by adjacent cells of the same type.

Figure 3.8: Summary of the boundary conditions applied to the unit cells developed for the shear set loading conditions. A full unit cell was simulated with the two X planes (marked in yellow dashed line) representing the periodic boundary conditions, while the bottom and the top of the cell are prescribed an encastre and a shear loading condition respectively. For each unit cell, the top view (left) and the perspective view (right) are shown.

3.3 Parametric optimisation

With the unit cell simulations set up, the 3D projected 4-polytope geometries were modified in an automated manner by parametrically manipulating the variables listed
in Table 3.1. This was achieved by defining the geometrical features of the computer-aided design (CAD) models in a Python script and having parametric design variables as inputs to the code that can be linked to the optimisation algorithm and automatically iterated. As a result, this enabled further exploration of the design space by means of an optimisation algorithm.

The 5, 8, 16 and 24-cell 4-polytope-based geometries were optimised for specific stiffness, \( \frac{E}{\rho} \), where \( E \) is the elastic modulus of the structure in axial compression and tension, and \( \rho \) is the apparent density of the structure. For the shear case, the objective was specific shear stiffness defined as \( \frac{G}{\rho} \), where \( G \) is the elastic shear modulus of the structure. This was achieved by combining the finite element simulations with an evolutionary algorithm based optimisation approach. The core of the framework is a single metamaterial unit cell simulation using the design parameters, described in Figure 3.2 and Table 3.1, as inputs for the FEA, and strain energy, \( U \), and mass of the total structure, \( m \), measures as outputs from the simulation. The optimisation algorithm adjusts the input design parameters and iterates the simulation process to determine the final structure exhibiting the highest specific stiffness or the highest specific shear stiffness. In its simplest form, this is expressed in Equation 3.1 for the axial loading and in Equation 3.2 for the shear loading scenario, where \( V \) is the total volume of the structure, \( m \) is the total mass of the structure, \( \sigma \) is the 1st Piola-Kirchhoff stress and \( U_e \) is the elastic strain energy.

\[
\max \frac{E}{\rho} = \left( \frac{\sigma^2 V}{2U_e} \right) \left( \frac{m}{V} \right)^{-1}
\]

\[
\max \frac{G}{\rho} = \left( \frac{\tau^2 V}{2U_e} \right) \left( \frac{m}{V} \right)^{-1}
\]

In order to calculate the specific stiffness values, Equation 3.3 was used to determine the elastic strain energy. Here, \( V_e \) is the volume of an element, \( n \) is the number of elements in a model, \( \sigma_{ij} \) is the stress tensor of an element, and \( \epsilon_{ij} \) is the elastic strain tensor of an element.

\[
U_e = \sum_{e=1}^{n} V_e \cdot \int_0^{\epsilon_{ij}} \sigma_{ij} d\epsilon_{ij}
\]

A single-objective GA was employed to avoid manual exploration of the design space. The parametric design variables for each consecutive generation of unit cell
3.3. PARAMETRIC OPTIMISATION

designs were based on the stored solutions of simulation results from preceding runs. The purpose of the GA was to find a unit cell arrangement demonstrating the highest specific stiffness properties in compression and tension cases and the highest specific shear stiffness in the shear loading case.

The process is completed when the objective function is realised which is defined by the strain energy and mass measure outputs from the FE simulations as these parameters are to determine the final value of $\frac{E}{\rho}$ for axial loading case (or $\frac{G}{\rho}$ for shear loading case). The process is iterated multiple times to assess the wide range of possible designs and to source the structure exhibiting the maximum $\frac{E}{\rho}$ (or $\frac{G}{\rho}$) value. The algorithm then makes use of the output from finite element analyses to evaluate the existing population of the metamaterial structures, selecting the best performing designs and subsequently using crossover and mutation to generate a new population. These steps were executed multiple times until a stop criterion was met and the near optimum design was found. A schematic flow diagram of the algorithm is shown in Figure 3.9.

Table 3.2: Summary of the parameters used in genetic algorithm set-up.

<table>
<thead>
<tr>
<th>GA parameters:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population size</td>
</tr>
<tr>
<td>Abs. no. of generations</td>
</tr>
<tr>
<td>Crossover probability</td>
</tr>
<tr>
<td>Mutation probability*</td>
</tr>
<tr>
<td>Crossover distribution index</td>
</tr>
<tr>
<td>Mutation distribution index</td>
</tr>
<tr>
<td>Stopping criteria</td>
</tr>
</tbody>
</table>

* $q$ is the number of design variables

The GA optimisation framework used a population size of 28, the choice of which was based on the number of genes, simulation complexity, and available parallel processing units. The absolute number of generations was not limited, however, the optimisation had a built-in stop-criterion which was activated when the results showed no improvement over the next 20% of the total generation number from the best solution. This stop-criterion reduced the computational costs of the optimisation and therefore reduce the design time. Each of the four structures presented reached the stop-criterion in under 756 design iterations. The crossover probability, mutation probability, and crossover and mutation distribution indices were set to 0.9, $\frac{1}{q}$, 10
3.3. PARAMETRIC OPTIMISATION

Figure 3.9: Schematic representation of genetic algorithm used in the optimisation framework.

and 20, respectively, where $q$ is the number of parametric design variables. GA parameter tuning was not carried out for this design problem as it was deemed beyond the scope of this work and the values were chosen to fit a universal design problem based on previously available knowledge [158]. The algorithm parameters chosen for this optimisation problem are summarised in Table 3.2.

Manufacturing constraints were incorporated to avoid exploring structures that could not be produced using the low force stereolithography (LFS) prototyping method. Two constraints were implemented, namely: (1) minimum thin wall thickness, which
was constrained by the force required to peel the print off the resin tank between each layer printing and (2) minimum drain hole diameter, which was limited by the resin viscosity to allow sufficient flow rate and hence draining of hollow chambers within the thin-walled structures. Therefore to reduce the overall computational time, structures with features that were too small to produce, or, which resulted in suction cups (concave features restricting resin flow around the printed part causing failed prints) were excluded from the design space exploration.

Specified ranges of design variables and the final values for optimised structures are presented in Appendix A with values for compression, tension and shear presented in Tables A.1, A.2 and A.3 respectively. The manufacturing approach is further discussed in Section 3.4.

3.4 Manufacturing

Considering the geometrical complexity of 4-polytope-based structures, additive manufacturing was chosen as the preferred fabrication method in this work. Recent advancements in this field have significantly reduced the cost of 3D printing technologies and increased the affordability of desktop additive manufacturing [34, 35, 36]. Nevertheless, out of the seven AM categories mentioned in Section 2.1.3 of Chapter 2, only two AM techniques, namely fused deposition modelling (FDM) (material extrusion category) and LFS (vat polymerisation category) were found to be affordable for this project.

The FDM method forms a 3D geometry by extruding a thermoplastic filament one layer at a time (along the horizontal plane) and is known to have significantly lower mechanical properties along the vertical direction in which the subsequent layers are formed. In fact, studies have shown that the variation in mechanical properties can be as high as 59.45% depending on the orientation of FDM printed parts [159, 160]. As this work focuses on developing mechanical metamaterials with similar in-plane and out-of-plane properties, the LFS method was chosen as the most suitable for manufacturing 4-polytope-based metamaterial samples. Limitations of this method, regarding the removal of residual resin inside the closed unit cells, were briefly discussed in Section 2.1.3 of Chapter 2 while the required unit cell design changes to accommodate for these limitations were presented in Section 3.1.1 of this chapter.
With the LFS chosen as the preferred method, the following paragraphs provide details on the sample fabrication approach.

Taking a more technical perspective, the experimental samples were manufactured using a photoreactive thermosetting resin (Clear V4) developed for LFS 3D printing by Formlabs. The samples were printed using a FormLabs Form 3 printer and the layer height was set to 25 µm. After the 3D printing process, the samples were washed in isopropyl alcohol using a Form Wash to ensure that uncured resin was removed. The samples were then post-cured in a Form Cure at 60°C in a UV light chamber for 30 minutes to increase the stability and strength of the parts, as suggested by the resin manufacturer.

The mass of the structures was consistent between the same geometry samples, however, these can vary between the different unit cell design samples due to areas of uncured or partially-cured resin not being accessible for washing as a result of the complex internal unit cell geometries. Accumulated resin that cannot be washed can therefore be cured during the post-curing process of the specimens, which can consequently increase the total mass of the structures and which may also alter the shape of the solid features. To circumvent this problem, the washing procedure was adjusted for each specimen type so as to minimise the resin residue inside the specimens. The mass variation, $\Delta w$, of the final cured specimens compared to the expected mass computed from the CAD model volumes was calculated as $\Delta w = \left(\frac{w_{\text{sample}}}{w_{\text{CAD}}} - 1\right)$, where $w_{\text{sample}}$ is the measured mass of the cured sample and $w_{\text{CAD}}$ is the calculated mass of the sample based on the computed CAD model volume and the cured density of Clear V4 resin.

The experimental samples of each of the three metamaterial sets, namely, compression, tension and shear, were manufactured using the same 3D printing method, 3D printing settings, and washing and post-curing procedures. Nevertheless, the experimental sample design, unit cell arrangement and sample mass variation results are different for each of the mentioned sets and therefore are further discussed in the dedicated manufacturing Sections 3.4.1, 3.4.2 and 3.4.3.

### 3.4.1 Compression sample manufacturing

The compression samples of the 4-polytope-based metamaterials were designed using the unit cells optimised for high specific stiffness under compressive loading, with the full boundary conditions described in Section 3.2.1. The unit cells were stacked
to create a cube-shaped compression sample made of an array comprising $5 \times 5 \times 5$ unit cells. Each specimen thence consisted of 125 unit cells and had the external dimensions of $50 \times 50 \times 50\text{mm}$. The samples were found to have high dimensional accuracy when compared against the CAD models, with a deviation of less than 0.3%. The mass variation, $\Delta w$, (first introduced in Section 3.4) was found to be 0.075, 0.076, 0.13 and 0.12 for the 5-cell, 8-cell, 16-cell and 24-cell samples, respectively.

![Figure 3.10: Representative compressive test specimens with a 5×5×5 3D projected 4-polytope unit cell array: (a) 5-cell, (b) 8-cell, (c) 16-cell and (d) 24-cell, and additional structures used as ‘comparative experimental controls’ also in a 5 × 5 × 5 array: (e) gyroid and (f) hexagonal honeycomb (tested in the out-of-plane direction).](image)

Sets of honeycomb and gyroid samples were additionally manufactured as a means of comparing the mechanical behaviour and properties of 3D projected 4-polytopes with more commonly researched cellular solid structures. The same resin and manufacturing technique was used as described for the 4-polytope-based structures, and representatives of each are shown in Figure 3.10. 3D printed honeycomb samples had a cell size of 8.5mm, wall thickness of 0.5mm, sample thickness of 30mm, volume fraction of 12.24% and an apparent density of 144 kg/m$^3$. These design variables were chosen to be in range of the apparent density (and thus closely associated geometrical parameters) of commercially available polymer honeycomb cores [101]. The gyroid samples were designed using a sinusoidal curve with an amplitude of 5.5mm...
3.4. MANUFACTURING

and period of 20mm. The wall thickness was 0.5mm, which resulted in a sample volume fraction of 7.68% and an apparent density of 89 kg/m$^3$. These parameters were based high performance gyroid structures in compression as reported in [3].

3.4.2 Tension sample manufacturing

The experimental samples of the tension set were designed using the appropriate unit cells optimised for high specific stiffness under tensile loading, with boundary conditions described in full in Section 3.2.2. The cells were stacked to create an array arrangement of $2 \times 2 \times 4$ with 16 unit cells in total and external sample dimensions of $30 \times 30 \times 120$mm. As shown in Figure 3.11, the unit cells in the middle section of the tensile sample ("test unit cells") are representative of the 4-polytope-based geometries designed using the optimisation framework while the cells adjacent to the middle section ("transition structure") have artificially higher wall thicknesses in comparison to the central unit cells. The ends of the sample were further reinforced by filling in the cavities with a two-part epoxy (RS Epoxy 406-9592). This ensured that the strength of the gripping area is sufficient to withstand the grip forces applied by the tensile testing machine. Such a design approach with three different areas within the tensile sample was chosen to mimic the "dog bone" geometry of the tensile coupons and hence maximise the chances of failure occurring within the central part of the specimen. An FE analysis was carried out to ensure that this coupon design does not impart any loads on the test unit cells when a force is applied to the gripping area.

All of the manufactured samples were found to have high dimensional accuracy with the deviation between the CAD models and the experimental samples being less than 0.42%. The mass variation, $\Delta w$, was found to be 0.1162, 0.0095, 0.1267, 0.1180 for 5, 8, 16 and 24-cell respectively.

In addition to the 4-polytope-based metamaterial samples, sets of gyroid and hexagonal honeycomb tensile samples were manufactured in an identical manner to carry out an experimental comparison of the mechanical properties between the 4-polytope-based structures and other commonly researched cellular solids. A sinusoidal wave with an amplitude of 3.75mm and a period of 30mm was used for the gyroid structure and the wall thickness was set to 0.85mm. The apparent density of the "test unit cells" within the gyroid tensile sample is 108.82 kg/m$^3$ while the relative density is 9.34%. The honeycomb tensile sample was made using hexagonal cells with
3.4. MANUFACTURING

Figure 3.11: Tensile specimen geometry designed to recreate the tensile behaviour of a “dog bone” shape coupon (black solid line). Main specimen areas: gripping (in purple), transition structure (in orange) and dedicated test unit cells (red dashed line).

Figure 3.12: Representative tensile test specimens with a $2 \times 2 \times 4$ 3D projected 4-polytope unit cell array. From left to right: 5-cell, 8-cell, 16-cell and 24-cell, and additional structures used as ‘comparative experimental controls’ - gyroid and hexagonal honeycomb (tested in the out-of-plane direction).

a diameter of 8.5mm and a wall thickness of 0.55mm which resulted in “test unit cells” with apparent and relative densities of 192.89 kg/m$^3$ and 16.56% respectively. The hexagonal geometry was aligned so that the out-of-plane direction of the cells is in line with the tensile loading direction, in order to obtain out-of-plane properties of the honeycomb sample. Both the gyroid and the hexagonal honeycomb tensile samples, were designed to have dedicated testing, transition and gripping areas as shown for the 4-polytope-based metamaterial samples in Figure 3.11. Representative
3.4. MANUFACTURING

tensile specimens of all of the 3D printed 4-polytope-based metamaterials, gyroid and hexagonal honeycomb structures are shown in Figure 3.12.

3.4.3 Shear sample manufacturing

Similar to compression and tension samples, the specimens for shear were designed using the unit cells optimised to show high specific stiffness under shear loading (boundary conditions presented in Section 3.2.3). The unit cell arrangement was chosen as $2 \times 2 \times 8$ to provide a sample size required for the mechanical testing procedure while fitting the build volume of the 3D printer. This resulted in a set of samples with 32 unit cells and external dimensions of $30 \times 30 \times 120$mm. The linear dimensional accuracy was evaluated by comparing the samples with the CAD models and the deviation value was determined to be less than 0.38%. The mass variation, $\Delta w$, was found to be 0.0534, 0.0790, 0.0506, 0.0910 for the 5-cell, 8-cell, 16-cell and 24-cell samples, respectively.

Figure 3.13: Representative shear test specimens with a $2 \times 2 \times 8$ 3D projected 4-polytope unit cell array. From left to right, 5-cell, 8-cell, 16-cell and 24-cell, and additional structures used as ‘comparative experimental controls’ - gyroid and hexagonal honeycomb.

Figure 3.13 illustrates all of the experimental shear samples, gyroid and honeycomb specimens which were also manufactured for comparison purposes. The gyroid structure was chosen due to the common research interest in the mechanical properties of this structure [3, 161] and the hexagonal honeycomb geometry was taken
3.5. MECHANICAL TESTING

as a structure which is widely adapted within the industry and is used as a go-to solution for lightweight sandwich panels [61, 162]. The geometrical parameters of the gyroid shape had a sinusoidal wave amplitude of 2.5mm and a period of 20 mm with a wall thickness of 0.5mm. The structure had an apparent density of 143.44 kg/m³ and a relative density of 12.32%. The honeycomb sample was made from hexagonal cells that closely mimic industrially available honeycomb core (CEL Components - PP8.120T30) [101] with a cell diameter of 8mm and a wall thickness of 0.55mm while the apparent and the relative densities for the sample were found to be 179.07 kg/m³ and 15.38% respectively. All of the unit cells within each of the shear samples were of the same geometry.

3.5 Mechanical testing

This section summarises the methodologies used for the mechanical characterisation of the three sets of metamaterial samples, namely, compression, tension and shear sets. The experimental testing procedures described here, summarise the axial loading in compression and tension as well as the shear loading using a 3-point bend test. The experimental results obtained using these methodologies are presented and analysed in Chapters 4, 5 and 6. In each loading case, five specimens, manufactured in the same manner, were tested for each of the 4-polytope-based metamaterials, as well as for each of the gyroid and honeycomb structures (tested out-of-plane). All samples were tested at a ramp rate of 10 mm/min, a rate at which cured neat resin exhibits Hookean behaviour under deformation. The rest of the mechanical testing details specific to each loading condition are summarised in the following sections.

3.5.1 Compressive testing set up

An Instron 3369 mechanical test machine with a load cell of 50kN (2530-50kN) was used to test the samples in compression between two horizontal compression platens. Strain measurements were taken using a 2D digital image correlation (DIC) technique (Imetrum system with 1400 × 1000 resolution at 17.8fps). Two axial strain measurements were taken across the flat outermost faces of the nine surface unit cells in the middle of the 5×5 metamaterial cell array, and were averaged to obtain strains in the axial direction (see Figure 3.14). The measurements were taken using the flat
3.5. MECHANICAL TESTING

faces in the same plane, located at the outermost surfaces of the specimen. This approach reduced the impact of free surface effects at the sample boundaries and hence, decreased the impact on the output strain values. It should be noted that the DIC system used has limitations as it is a 2D measurement technique, and hence does not capture internal or out-of-plane deformations.

![Figure 3.14](image)

**Figure 3.14:** Two vertical strain measurements were taken across the flat features in the same plane, located at the outermost surfaces of the specimen in the middle of the 5 × 5 metamaterial cell array ((a)–(d)). Similarly, the strains of the hexagonal honeycomb (e) and gyroid (f) were measured using the flat outermost surfaces and flat features on these surfaces. The strain values (strain 1 & strain 2) were averaged to obtain the overall strain of a specimen. The same strain measurement approach was used for tension and shear metamaterial sets.

### 3.5.2 Tensile testing set up

An Instron 8802 servo-hydraulic test machine mounted with a 250kN load cell (2742-501) and tensile grips for samples up to 32mm in diameter was used for testing specimens in tension. An Imetrum 2D digital image correlation (DIC) system (resolution of 1400 × 1000 at 17.8fps) was employed for taking two axial strain measurements across the four outermost faces of the unit cells situated in the middle of 2 × 4 metamaterial array within the tensile specimen. This 2D image correlation technique
allowed for measurements to be taken in the axial direction, which were then averaged to obtain the final strain measurement values.

### 3.5.3 Shear testing set up

The set of metamaterials optimised for shear was mechanically tested using the same test frame as described in Section 3.5.1. The shear loading conditions were recreated using the Instron 3369 mechanical test machine, a load cell of 10kN (2530-10kN) and a 3-point bend fixture with a maximum specimen width of 40 mm. The strain measurements were taken with the 2D digital image correlation equipment (Imetrum DIC system with 1400 × 1000 resolution at 17.8fps) to track the deflection in the middle of the sample caused by the downward crosshead movement with respect to the stationary support pins located at the bottom of the sample. The effective span-to-depth ratio of 2 was chosen to ensure that the specimen strength is representative of its structural shear properties [163].
Chapter 4

Properties of the compressive metamaterial set

This chapter builds on the design, optimisation and manufacturing methodology discussed in Chapter 3 and focuses on discussing the 4-polytope-based metamaterials developed for compressive loading applications. It presents simulation results as well as experimental findings while considering the accuracy of simulations and identifying limitations of the experimental work. The compressive 4-polytope-based structures are compared to other commonly researched structures such as gyroid and hexagonal honeycomb structures in terms of mechanical performance. In addition, the 4-polytope internal geometry effect on relative consistency of mechanical properties is discussed and compared showcasing the strength gain due to internal metamaterial architecture rather than bulk material properties. The work presented in this chapter was published in [155]. Progressive optimisation outputs for compressive metamaterial structures are illustrated in Figure B.1 of Appendix B while the full dataset is also available on the Edinburgh Data Share website [20].

4.1 Simulation results

As discussed in Section 3.2, Chapter 3, the simulation-based optimisation framework generated a set of metamaterial structures for each 3D projected 4-polytope geometry. The final values for optimised structures are provided in Table A.1 as a part of Appendix A. The performance of each was assessed and ranked according to the objective function, which evaluated the specific stiffness of each structure. Figure
4.1 summarises the performance of four sets of 4-polytope-based geometries and illustrates the incremental progression of each at different stages of the optimisation process. The colours in the bar chart represent the specific stiffness of (i) an unoptimised structure (0% of the total optimisation), (ii) 33% of the total optimisation, (iii) 67% of the total optimisation and (iv) a fully optimised structure (100% of the total optimisation). As the algorithm explores the design space, the specific stiffness of the structures can be seen to increase for each of the 3D projected 4-polytopes. The performance enhancement between the unoptimised and fully optimised structures are 64.74%, 38.40%, 137.12% and 78.18% for the 5-cell, 8-cell, 16-cell and 24-cell metamaterial structures. The metamaterial structure with the highest specific stiffness at 100% of the total optimisation is found to be the 8-cell, followed by the 5-cell, 16-cell and 24-cell, in that order. Since the 8-cell also has the lowest level of post-optimisation improvement when compared to the other structures, it shows that the 3D projected tesseract is already a highly advanced 3D projection with excellent properties of stiffness against density.

![Figure 4.1: Increases in specific stiffness with incremental optimisation progression from the unoptimised (0%) to the fully-optimised (100%) iteration for 24, 16, 5 and 8-cell metamaterial structures, in that order.](image)

To better understand these results, the strain energy density was assessed in relation to the overall energy storage capacity of each 3D projected 4-polytope structure over the optimisation process. Figure 4.2 shows the 5-cell, 8-cell, 16-cell and 24-cell structures at (i) 0% (ii) 33% (iii) 67% and (iv) 100% of the total optimisation. The colour map illustrates the distribution of elastic strain energy density within each
4.1. SIMULATION RESULTS

Figure 4.2: Comparison of optimised 4-polytope-based structure models with labels (i) to (iv) representing optimisation level: 0% (unoptimised), 33%, 67% and 100% (fully-optimised) structures, respectively. The colour map shows the elastic strain energy density (ESEDEN) distribution in J/cm$^3$ at the compression strain of 0.08 in each structure.

structure and indicates the geometrical regions of each structure that contribute the most towards load-bearing under axial compression. Strain energy can be seen to distribute through more of the solid state continuum from the unoptimised structures through to the fully optimised structures. As such, the total stored elastic strain energy increases for each structure with respect to the increasing level of geometrical optimisation. As the ability to store elastic strain energy correlates directly with
metamaterial stiffness, the fully optimised structures consequently exhibit the highest stiffness values. When factored against their final apparent densities, we find that the fully-optimised structures in each set also have the highest specific stiffness values within each set as shown previously in Figure 4.1. The fully-optimised structures that distribute strain energy more effectively through the solid state continuum of each structure (5-cell and 8-cell) also absorb higher levels of elastic strain energy and this contributes to their higher (homogenised) compressive modulus and thus higher (homogenised) specific stiffness values. Structures with more localised strain energy (16-cell and 24-cell) have comparatively lower (homogenised) specific stiffness values. This is related to the effectiveness in the distribution of elastic strain energy through a greater volume of the body of the material, which is therefore a key design consideration as it contributes towards the overall stiffness of the structure. Structures comprising lower levels of internal geometrical complexity (5-cell and 8-cell) are noticeably more resistant to compressive loading than more complex structures (16-cell and 24-cell). This is primarily because 3D projected 4-polytope metamaterials with higher levels of geometrical complexity have more slender edges and sharper corner features. This combination of geometrical features results in the localisation of higher strain energies at lower loads.

4.2 Experimental testing results

4.2.1 Specific stiffness and yield strength properties

Figure 4.3 plots the experimentally measured specific stiffness values against experimental specific yield strength values for each of the 3D projected 4-polytopes. The arithmetic mean of each specific property is shown based on five specimens tested for each structure \( n = 5 \), and the vertical and horizontal bars represent the total range of measured experimental values for each measured property. To enable comparison with more common structures, the chart includes the data points for the 3-dimensional cubically symmetrical gyroids, and the hexagonal honeycomb structures (tested out-of-plane), which were manufactured in the same way as the 4-polytope-based metamaterials (cf. Section 3.4, Chapter 3). In this figure, 3D projected 4-polytopes follow the same trend as has been predicted by the simulations. The 8-cell metamaterials exhibit the highest specific stiffness with an average value of 0.68 MNm/kg, followed by the 5, 16 and 24-cell metamaterials, which have average values of 0.43, 0.28 and
4.2. EXPERIMENTAL TESTING RESULTS

0.19 MNm/kg, respectively. The experimental results furthermore indicate that the specific yield strength values follow a similar trend with the 8-cell metamaterials having the highest value of 22.8 kNm/kg, followed by the 5-cell, 16-cell and 24-cell metamaterials. Metamaterial designs with (a) less complex internal structures and (b) geometric features more closely in-line with the direction of loading, perform noticeably better in terms of specific stiffness and specific yield strength. Such a trend aligns well with the strain energy density results summarised in Figure 4.2, which showed that the structures with a less distributed strain energy density have a lower overall capacity to store strain energy and hence exhibit a lower overall stiffness.

![Figure 4.3: Comparison of experimental results of 4-polytope-based metamaterials to honeycomb and gyroid structures (n = 5).](image)

Figure 4.3 also demonstrates that each of the 3D projected 4-polytope metamaterials outperform a cubically symmetric 3D gyroid in terms of both specific stiffness and specific yield strength. All structures exhibit a lower specific stiffness than a hexagonal honeycomb tested in the out-of-plane direction, however, it should also be noted that there is overlap between the 8-cell and honeycomb error bars and as such the best of the experimental 8-cell metamaterials are as high in specific stiffness
as the least of the honeycomb structures tested out-of-plane. In addition, the 8-cell tesseract outperforms the hexagonal honeycomb by 17.3% in terms of its specific yield strength. This is because the 8-cell metamaterial has thin-walled features oriented in the axis of loading, in a similar manner to those of the hexagonal honeycomb when loaded in an out-of-plane direction. An arrangement of this kind benefits both the overall stiffness and strength of a structure and additionally, the optimised geometry of the 8-cell metamaterial minimises any internal stress concentrations. The combination of the two aforementioned factors is plausibly the reason for why the 8-cell metamaterial has such a high specific yield strength. One significant difference between the 3D projected 4-polytope metamaterials and the out-of-plane honeycomb, is that the 4-polytope-based metamaterials have the same mechanical properties in all three orthogonal axes (i.e. they are cubically symmetric). This is highly dissimilar to the honeycomb structures, which are essentially 2D hexagonal packings extruded orthogonally in a 3rd axis. While they have a very high specific stiffness in the out-of-plane direction, they are also very weak and of low stiffness in their in-plane axes, deforming significantly when loaded in-plane [116].

Table 4.1: Mean specific stiffness \( \bar{E}/\rho \) results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures and specific stiffness values \( \bar{E}/\rho \) for simulated models: 5, 8, 16 and 24-cell metamaterials.
4.2. EXPERIMENTAL TESTING RESULTS

Table 4.2: Mean specific yield strength \( \left( \frac{\sigma_y}{\rho} \right) \) results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures, and specific strength values \( \left( \frac{\sigma_y}{\rho} \right) \) for simulated models: 5, 8, 16 and 24-cell metamaterials.

<table>
<thead>
<tr>
<th>Experimental</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean specific yield strength ( \left( \frac{\sigma_y}{\rho} \right) ), (kNm/kg)</td>
<td>12.62</td>
<td>22.80</td>
<td>7.16</td>
<td>6.28</td>
<td>5.72</td>
<td>19.43</td>
</tr>
<tr>
<td>Upper value</td>
<td>13.59</td>
<td>25.58</td>
<td>7.69</td>
<td>6.65</td>
<td>5.86</td>
<td>22.95</td>
</tr>
<tr>
<td>Lower value</td>
<td>10.62</td>
<td>19.32</td>
<td>6.72</td>
<td>5.53</td>
<td>5.46</td>
<td>16.96</td>
</tr>
<tr>
<td>Median</td>
<td>13.57</td>
<td>22.73</td>
<td>7.17</td>
<td>6.41</td>
<td>5.81</td>
<td>19.22</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>1.226</td>
<td>2.046</td>
<td>0.383</td>
<td>0.417</td>
<td>0.152</td>
<td>2.032</td>
</tr>
<tr>
<td>CoV</td>
<td>9.7%</td>
<td>9.0%</td>
<td>5.4%</td>
<td>6.6%</td>
<td>2.7%</td>
<td>10.5%</td>
</tr>
</tbody>
</table>

| Simulations | | | | | | |
| Specific yield strength \( \left( \frac{\sigma_y}{\rho} \right) \), (kNm/kg) | 15.76 | 25.28 | 9.29 | 7.90 | N/A | N/A |
| Percentage diff. (sim. vs exp.) | 20.0% | 9.8% | 22.9% | 20.5% | N/A | N/A |
| Z-score | 2.56 | 1.21 | 5.57 | 3.89 | N/A | N/A |

Tables 4.1 and 4.2, provide experimental and simulation results for specific stiffnesses and specific yield strengths, respectively. Statistical details are included for the experimental phases of the work (experimental range, standard deviation and the coefficient of variance (CoV)), and a comparison is also made between the simulation results for each sample set as a percentage difference and a Z-score \( (Z) \), where in the case of specific stiffness, \( Z = \frac{E - \bar{E}}{S} \) and in the case of specific yield strength, \( Z = \frac{\sigma_y - \bar{\sigma_y}}{S} \), and \( S \) is the standard deviation of the sample set. From these tables, we note that the simulations are overall between 18.9% and 28.2% different from the arithmetic mean of the sample sets when comparing for specific stiffness, and between 9.8% and 22.9% different from the arithmetic mean of the sample sets when comparing for specific yield strength. The Z-scores range between 2.88 and 8.33, and 1.21 and 5.57 when comparing between simulation and experiment for specific stiffness and specific yield strength, respectively. The simulated specific yield strength results are also the most accurate for the 8-cell metamaterial with the percentage difference from the experimental results being 9.82%, while the values for the 5-cell, 16-cell and
4.2. EXPERIMENTAL TESTING RESULTS

24-cell were found to be 19.95%, 22.94% and 20.51% respectively. Following the same trend, the 8-cell-based structure has the lowest Z-score value of 1.21 while the 16-cell has the highest value of 5.57. The 8-cell structures have the lowest Z-score in each case (2.88 and 1.21) indicating that the 8-cell manufactured samples are the closest in properties to the properties predicted through simulation.

Figure 4.4 shows how the simulated stress-strain curves for each of the 4-polytope-based structures tend to lie closer to the upper bound of the experimental ranges in each sample set. While the stress-strain curves of the 8-cell, 16-cell and 24-cell simulations are reasonably close to the experimental curves, the 5-cell simulations are less correlated with the experimental test results. Reasons for why the experimental stress-strain curves are generally slightly lower than the simulation curves most likely originates from limitations related to specimen manufacture. As discussed in Section 3.4, Chapter 3, the specimen mass was found to be higher than the model mass due to surplus resin that accumulated within the 3D printed structures. Inconsistencies in resin deposition are a plausible cause for unpredicated stress distributions leading to the development of stress concentrations. In addition to this, since in the post-curing process, samples are exposed to heat and UV light to increase the cross-linking of the polymer, the post-curing rate of each 4-polytope-based structure is unique, as curing is affected by the distinctive geometry of a structure, and its surface area to volume ratio. As such, there are variable levels of curing not only within individual samples, but also between the different sample sets. Variability between the samples is obvious from the experimental results in Figure 4.4 and since the simulation results represent fully cured, and ideally cured structures, the simulation predictions will naturally tend towards a more mechanically ideal upper bound from the experimentally measured samples. The limitations of 2D digital image correlation system (previously discussed in Section 3.5.1, Chapter 3) are also considered to contribute towards the experimental errors and plausibly the difference between simulation and experimental results. The effects of the out-of-plane deformation of features within the metamaterial structures could not be evaluated using this technique and a 3D DIC system could be an improvement in terms of future work.

4.2.2 Effect of optimisation on other mechanical properties

The specific properties discussed thus far have been achieved by means of maximising the elastic energy stored in each of the 4-polytope-based structures. Ascertaining how
4.2. EXPERIMENTAL TESTING RESULTS

Figure 4.4: Upper and lower experimental bound stress-strain curves, and simulation stress-strain curves for 5-cell, 8-cell, 16-cell and 24-cell 4-polytope-based structures.
a focus on strain energy optimisation might also impact other mechanical properties is a worthwhile exercise, as it allows for the further comparison of 4-polytope-based metamaterials over a wider range of mechanical properties.

Representative compressive stress-strain curves from each of the experimental tests are provided in Figure 4.5 and the following properties are compared in Table 4.3: Young’s modulus (in compression), yield strength, compressive strength, modulus of resilience, and the modulus of toughness. The standard deviation (SD) and the coefficient of variation (CoV) are also provided for each property in each sample set. The experimental 8-cell metamaterial samples exhibit the highest mean Young’s modulus out of all of the sample sets at 145.01 MPa. This is 12.6% higher when
4.2. EXPERIMENTAL TESTING RESULTS

Table 4.3: Summary of experimentally obtain mechanical properties: Young’s modulus (compression), yield and compressive strength, modulus of resilience and modulus of toughness for 4-polytope-based metamaterials, and for gyroid and hexagonal honeycomb structures.

<table>
<thead>
<tr>
<th></th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s m., (MPa)</td>
<td>70.53</td>
<td>145.01</td>
<td>43.52</td>
<td>11.73</td>
<td>15.30</td>
<td>128.75</td>
</tr>
<tr>
<td>SD</td>
<td>3.59</td>
<td>14.21</td>
<td>4.36</td>
<td>0.39</td>
<td>0.13</td>
<td>14.38</td>
</tr>
<tr>
<td>CoV</td>
<td>5.09%</td>
<td>9.80%</td>
<td>10.01%</td>
<td>3.37%</td>
<td>0.85%</td>
<td>11.17%</td>
</tr>
<tr>
<td>Yield strength, (MPa)</td>
<td>2.09</td>
<td>4.90</td>
<td>1.13</td>
<td>0.38</td>
<td>0.51</td>
<td>2.80</td>
</tr>
<tr>
<td>SD</td>
<td>0.20</td>
<td>0.44</td>
<td>0.06</td>
<td>0.03</td>
<td>0.01</td>
<td>0.29</td>
</tr>
<tr>
<td>CoV</td>
<td>9.72%</td>
<td>8.97%</td>
<td>5.35%</td>
<td>6.64%</td>
<td>2.66%</td>
<td>10.46%</td>
</tr>
<tr>
<td>Comp. strength, (MPa)</td>
<td>3.47</td>
<td>5.91</td>
<td>1.22</td>
<td>0.44</td>
<td>0.65</td>
<td>3.95</td>
</tr>
<tr>
<td>SD</td>
<td>0.28</td>
<td>0.56</td>
<td>0.05</td>
<td>0.01</td>
<td>0.01</td>
<td>0.44</td>
</tr>
<tr>
<td>CoV</td>
<td>8.14%</td>
<td>9.45%</td>
<td>3.79%</td>
<td>3.33%</td>
<td>1.04%</td>
<td>11.12%</td>
</tr>
<tr>
<td>M. of resilience, (kJ/m³)</td>
<td>53.50</td>
<td>95.32</td>
<td>14.37</td>
<td>7.88</td>
<td>6.29</td>
<td>27.95</td>
</tr>
<tr>
<td>SD</td>
<td>12.30</td>
<td>11.97</td>
<td>2.44</td>
<td>1.01</td>
<td>1.09</td>
<td>4.40</td>
</tr>
<tr>
<td>CoV</td>
<td>22.99%</td>
<td>12.56%</td>
<td>17.02%</td>
<td>12.85%</td>
<td>17.26%</td>
<td>15.74%</td>
</tr>
<tr>
<td>M. of toughness, (kJ/m³)</td>
<td>130.21</td>
<td>294.50</td>
<td>32.04</td>
<td>14.52</td>
<td>48.62</td>
<td>239.16</td>
</tr>
<tr>
<td>SD</td>
<td>14.48</td>
<td>32.71</td>
<td>7.57</td>
<td>1.43</td>
<td>10.50</td>
<td>37.43</td>
</tr>
<tr>
<td>CoV</td>
<td>11.12%</td>
<td>11.11%</td>
<td>23.62%</td>
<td>9.84%</td>
<td>21.60%</td>
<td>15.65%</td>
</tr>
</tbody>
</table>

compared against the mean Young’s modulus of the hexagonal honeycomb, which was 128.75 MPa out-of-plane. The 5-cell and 16-cell based metamaterials outperform the gyroid samples exhibiting mean Young’s modulus values of 70.53, 43.52 and 15.30 MPa, respectively. The structure with the lowest stiffness out of the 4-polytope-based geometries is the 24-cell, which has a mean Young’s modulus of 11.73 MPa. The CoV ranges between 0.85% and 11.17% for all sample sets, and demonstrates a high level of consistency in the experimentally measured Young’s modulus values in each of the sample sets.

Similar trends are evident when observing the mean yield and compressive strength properties. Here, the 8-cell metamaterial exhibits the highest mean yield and compressive strength values at 4.90 MPa and 5.91 MPa, respectively. The yield strength value is 175% higher and the compressive strength is 150% higher when compared against the hexagonal honeycomb tested out-of-plane, which yields on average at 2.80 MPa and reaches a maximum compressive strength on average at 3.95 MPa. The 5-cell and 16-cell yield and compressive strengths surpass those of the gyroid, while the
24-cell metamaterial, which also has the lowest apparent density, is the weakest of the six structures under scrutiny.

The experimental data additionally suggests that the 8-cell followed by the 5-cell metamaterials, have a higher ability to absorb elastic energy when compared against the hexagonal honeycomb samples, outperforming the latter by 3.4 and 1.9 times, respectively. When compared to the 3-dimensional gyroid, all of the 4-polytope-based metamaterials exhibit a higher modulus of resilience, demonstrating the suitability of these structures in applications where elastic energy storage in compression is a key design consideration. Nevertheless, as compressive loading increases beyond the elastic limit, the 4-polytope-based metamaterials display a relatively short plastic region when compared to that of the honeycomb and gyroid structures. Moreover, the plastic regions of the 4-polytope-based metamaterials are coupled to catastrophic failure soon after reaching maximum compressive strength. As such, the 4-polytope-based metamaterials are significantly more brittle than the honeycomb and gyroid structures, which is in turn an artifact of an optimisation process that favoured elastic energy storage. It can therefore be inferred that maximising the elastic strain energy storage capacity of a metamaterial concurrently minimises its ability to gradually release energy through plastic deformation and as such, catastrophic failure is an expected mechanical behaviour that is borne through the optimisation process.

Finally, the modulus of toughness is highest in the 8-cell metamaterial (294.50 kJ/m$^3$), followed by the hexagonal honeycomb (239.16 kJ/m$^3$). The 5-cell metamaterial fails at the strain of 0.074 and has a modulus of toughness of 130.21 kJ/m$^3$, which is higher 2.68 times higher than that for a gyroid over its complete 0.08 strain range. The toughness values for 16-cell and 24-cell metamaterials are significantly lower (32.04 and 14.52 kJ/m$^3$, respectively). This is ultimately a consequence of sample fracture at low strain values. The 16-cell metamaterials failed on average at a strain of 0.04, while the 24-cell metamaterials failed at an average strain of 0.055.

### 4.2.3 Performance comparison with existing mechanical metamaterials

In Figure 4.6 the compressive strength normalised by the bulk Young’s modulus of fully cured solid resin is plotted against the relative density of the sample provided in Table 4.4. This is a normalisation method by which means the strength gain of metamaterials can be visualised [164]. In this figure, the data points are plotted
4.2. EXPERIMENTAL TESTING RESULTS

Figure 4.6: The compressive strength normalised by bulk Young’s modulus plotted against the relative density of the sample - the data points are plotted against generalised area plots for different metamaterial structures at the nano, micro and macro length scales.

Table 4.4: Apparent and relative densities of simulated and experimentally tested samples.

<table>
<thead>
<tr>
<th></th>
<th>Simulations</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apparent density, (kg/m$^3$)</td>
<td>Relative density</td>
</tr>
<tr>
<td>5-cell</td>
<td>154.00</td>
<td>13.22%</td>
</tr>
<tr>
<td>8-cell</td>
<td>199.48</td>
<td>17.12%</td>
</tr>
<tr>
<td>16-cell</td>
<td>139.24</td>
<td>11.95%</td>
</tr>
<tr>
<td>24-cell</td>
<td>54.65</td>
<td>4.69%</td>
</tr>
<tr>
<td>Gyroid</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Hex honeycomb</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

against generalised area plots for different metamaterial structures at the nano, micro and macro length scales, based on data from [164]. Honeycomb structures tested...
4.2. EXPERIMENTAL TESTING RESULTS

in the out-of-plane direction are generally expected to display a high normalised compressive strength at relatively low densities, and this is observed in Figure 4.6, where the (macro-scale) honeycomb is at a level that is typically a lower level of nanostructures, which themselves ordinarily have normalised strengths above those of macro-structures. Noting this, it can also be observed that the (macro-scale) 8-cell metamaterials have higher normalised strength and relative density values than the honeycomb structures, while 5-cell metamaterials are similar to honeycombs. Contrarily, the gyroid and 24-cell metamaterials exhibit a notably lower normalised strength with respect to their relative densities, while the 16-cell metamaterials show fairly typical properties for generic macro-structures such as macrolattices.

The stiffness and strength properties discussed in the sections above can also be related to the relative density or porosity of 4-polytope-based metamaterials. Choi and Lee [122], provide the only report detailing relationships between the porosity and stiffness, and the porosity and strength of hypercubes, or, tesseracts. In their work, they discuss the strength and stiffness of strut-based hypercubes in terms of 

\[
\left( \frac{E^*}{E_s} \right) = C \left( \frac{\rho^*}{\rho_s} \right)^a \quad \text{and} \quad \left( \frac{\sigma^*}{\sigma_s} \right) = D \left( \frac{\rho^*}{\rho_s} \right)^b,
\]

respectively, where \( E, \sigma \) and \( \rho \) are the Young’s modulus, the strength in compression and the density, respectively. The symbols * and s represent the hypercube including pore space, and the bulk constituent solid material, respectively. They hypothesise that the strength and stiffness of strut-based hypercubes (i.e. strut-based tesseracts) can be represented using the empirical formulas and conclude that in hypercubes where the pore space is unfilled, \( a = b = 1.11 \) and \( C = 0.023 \) while \( D = 0.01 \).

Table 4.5: Calculations of constants \( C \) and \( D \) using experimental data in Tables 4.3 and 4.4.

<table>
<thead>
<tr>
<th></th>
<th>( C )</th>
<th>( D )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-cell</td>
<td>0.30</td>
<td>0.25</td>
</tr>
<tr>
<td>8-cell</td>
<td>0.45</td>
<td>0.44</td>
</tr>
<tr>
<td>16-cell</td>
<td>0.20</td>
<td>0.14</td>
</tr>
<tr>
<td>24-cell</td>
<td>0.15</td>
<td>0.14</td>
</tr>
<tr>
<td>Gyroid</td>
<td>0.13</td>
<td>0.12</td>
</tr>
<tr>
<td>Honeycomb</td>
<td>0.65</td>
<td>0.39</td>
</tr>
</tbody>
</table>

Taking the mean values of Young’s modulus and yield stress from Table 4.3 as inputs for \( E^* \) and \( \sigma^* \), the experimental relative densities from Table 4.4 as input values for \( \frac{\rho^*}{\rho_s} \), and \( a = b = 1.11 \), the \( C \) and \( D \) constants are calculated and shown for each
4.3. KEY FINDINGS

of the structures in Table 4.5. The $C$ and $D$ constants provide value as they allude to residual stiffness and strength, respectively, as reduced stiffnesses and strengths from a solid block of material due to the presence of pore space. There is a large difference between $C$ and $D$ for the honeycomb structures, which indicates that while these structures are superior in terms of stiffness ($C = 0.65$), they lose significant mechanical value when it comes to strength ($D = 0.39$), and this may be due to how honeycombs will buckle causing an onset of plastic straining, after which they crumble. 5-cell and 16-cell metamaterials also display notable differences between $C$ and $D$ constants however, these are not as extreme as in honeycomb structures. Both 8-cell and 24-cell metamaterials, as well as gyroids, retain relative closeness between their $C$ and $D$ constants, indicating that both strength and stiffness are equally reduced from the bulk material properties due to pore space. Nevertheless, the optimised 8-cell metamaterial structures have significantly higher $C$ and $D$ constants than have previously been reported [122] exceeding the previous constants for tesseracts by ca. 20-fold and 44-fold in terms of stiffness and strength, respectively. It should be nevertheless be noted that the properties of mechanical metamaterials are governed by architecture, length scale and material composition as affected by the manufacturing, in parallel [164]. As such, the comparisons made herein are primarily to showcase how 3D projected 4D geometries compare in terms of residual strength and stiffness as reduced through the presence of pore space. What we find here therefore, is that architecture has a profound effect on the relative consistency of properties. Cubically symmetric structures display the greatest levels of consistency in terms of both strength and stiffness reductions from the presence of unfilled, empty spaces (porosity), while of these, tesseract (8-cell), octaplex (24-cell) and gyroid structures are the most consistent.

4.3 Key findings

This chapter summarises, the use of 3D projected 4D geometries (4-polytopes) as a basis for a metamaterial set designed and optimised for compressive loading. The evidence presented here demonstrates that this new class of mechanical metamaterial has considerable potential as cubically symmetrical structures with superior properties of specific stiffness and strength. While such structures have the obvious benefit of being enablers of multi-directional mechanical resistance, certain forms e.g. 8-cell
(tesseract) and 24-cell (octaplex) structures, reduce equally from the original bulk properties in terms of strength and stiffness, with respect to pore-space. This characteristic is not seen in more common honeycomb structures, though it is evident in gyroids, most plausibly because the gyroids are also cubically symmetric.

Genetic algorithms coupled with parametric optimisation have improved the properties of specific stiffness of 4-polytope-based structures by ca. 65%, 38%, 137% and 78% for 5-cell (pentatope), 8-cell (tesseract), 16-cell (orthoplex) and 24-cell (octaplex) metamaterials. Nevertheless, only certain structures amongst the optimised 4-polytope-based geometries show significant promise in terms of their final properties. In particular, the optimised 8-cell tesseract has a higher specific yield strength than even hexagonal honeycomb structures loaded in the out-of-plane direction, and their specific stiffness values are within the same range of values measured for the honeycombs. Both the 8-cell tesseract as well as the 5-cell pentatope, in similitude to the honeycomb structures, have very high normalised compressive strengths and lie within the range of values for nanolattice-based metamaterials when plotted against their relative densities, the 8-cell tesseract being the highest of the three aforementioned structures.

The optimisation methodology and corresponding results evidence that there is validity and significance in developing advanced mechanical metamaterials from 3D projected 4-polytopes. The parametric design approach in combination with the genetic algorithm based optimisation used herein, demonstrates that mechanical performance can be enhanced whilst maintaining lightweightness. The cubically symmetrical nature of 4-polytope-based structures offers great advantages for maintaining structural stiffness for multi-axial loading, which is beneficial in many real-life applications.
Chapter 5

Properties of the tensile metamaterial set

This chapter presents 4-polytope-based metamaterials designed to exhibit high specific stiffness properties under tensile loading. Similarly to the compression set in Chapter 4, the tensile set was put through the simulation, optimisation and manufacturing methodology discussed in Chapter 3. The simulation outputs for the tensile metamaterial set are shown at the beginning of the chapter, followed by experimental results. Additionally, the impact of optimisation on mechanical tensile properties is analysed and the performance of the developed metamaterials is evaluated against the gyroid and honeycomb structures. The work presented in this chapter was published in [156]. Progressive optimisation outputs for tensile metamaterial structures are shown in Figure B.2 of Appendix B, the full dataset is also made available on the Edinburgh Data Share website [21].

5.1 Simulation results

The 4-polytope-based geometries were developed using the simulation-based approach described in detail in Chapter 3. 3D projected 5-cell, 8-cell, 16-cell and 24-cell 4-polytopes were designed with the aim of maximising specific stiffness. An optimisation framework was used to automate exploration of the design space, which monitored incremental improvements in specific stiffness with each new structure generated. As the mass and hence the relative density of each iteratively generated design could not be the same due to the high number of parametric design variables, a specific property was chosen as the performance metric in this optimisation study.
5.1. SIMULATION RESULTS

Figure 5.1: Specific stiffness comparisons between the 5, 8, 16 and 24-cell 3D projected 4-polytopes from unoptimised (0%) to fully optimised (100%) showing 25% increments of progression in the optimisation process.

Figure 5.1 illustrates the improvements in specific stiffness at 0% (no optimisation), 25% of optimal, 50% of optimal, 75% of optimal and 100% (full optimisation) of each 3D projected 4-polytope in tension. The maximum improvement in specific stiffness through our optimisation framework are 121.79%, 72.45%, 163.44% and 468.71% for 5-cell, 8-cell, 16-cell and 24-cell metamaterials, respectively. The 8-cell metamaterial structure has a specific stiffness that at 0% optimisation, is greater than the fully optimised 5-cell, 16-cell and 24-cell structures. It has therefore, a base cellular architecture that is already notably higher-performance when compared against the other 3D projected 4-polytopes researched here. It also exhibits the lowest percentage increase from its unoptimised to its fully optimised states, while the 5-cell, 16-cell and 24-cell, as a percentage improvement from a base structure, can be seen to benefit significantly more through the optimisation framework, clarifying that adjustments of parametric design variables can yield a wide range of metamaterial architectures with improved properties of specific stiffness.

Figure 5.2 shows the elastic strain energy density for each of the 3D projected 4-polytope metamaterials at different levels of optimisation starting at unoptimised (0%) to fully optimised (100%). These plots show that strain energy density increases within each metamaterial structure as a function of increased levels of structural optimisation. As such, each unit cell type (5, 8, 16 and 24-cell) can be seen to develop
5.1. SIMULATION RESULTS

Figure 5.2: Color maps for each of the 3D projected 4-polytope metamaterials. Each column illustrates the progress in optimisation at the following different stages: (i) 0% (unoptimised), (ii) 25%, (iii) 50%, (iv) 75% and (v) 100% (fully optimised). The colour legend represents the elastic strain energy density (ESEDEN) values in J/cm$^3$ and the cells are loaded in tension to 2% strain.

A higher overall capacity to store elastic strain energy when loaded in tension, as the structure is progressively optimised. Since the capacity to store strain energy is also related to the overall elastic modulus of each structure, the unit cells with the most evenly distributed strain energy densities gain the highest stiffness. The plots furthermore enable the identification of regions within each metamaterial unit cell that contribute the most towards strain energy absorption and thus the overall stiffness. Nevertheless, the broader objectives were not only to optimise the structure for stiffness, but also for lightweightness. This was achieved using a coupled objective as discussed in Section 3.3 of Chapter 3. When the apparent density is thence taken into account, the fully-optimised structures for each of the 3D projected 4-polytope types, have the highest specific stiffness values as previously shown in Figure 5.1. Visually,
the most effective strain energy density distribution is in the fully-optimised 8-cell structure, followed by the 5-cell and 16-cell structures. The structure with the most localised strain energy density, namely 24-cell, has the lowest capacity for storing strain energy and hence the lowest specific stiffness. This is due to the fact that the high strain energy density levels concentrated in a single location tend to cause early local failures within the structure under tensile loading, lowering therefore, the limit of elastic proportionality in these structures. Similar findings regarding truss metamaterial failure at the locations within the structure with high strain energy density values were reported by Bhuwal et al. [165]. As such, the optimal structures are the ones that are able to share strain energy most effectively throughout the larger volume of a unit cell. This can therefore be seen as a fundamental design consideration in high stiffness mechanical metamaterials. In the case of our 3D projected 4-polytopes, this can in turn, be directly correlated to the geometrical complexity of each of the structures. The best-performing 8-cell metamaterial has the lowest levels of geometrical complexity, followed by the 5-cell and 16-cell, whereas the 24-cell, which is the least optimal in terms of performance within the range of linear elasticity, is geometrically most complex. Structures with a higher level of geometrical complexity tend to have higher numbers of sharp features, such as corners and slender edges, and this results in more points within the structure where strain energy localisation occurs.

5.2 Experimental results

5.2.1 Specific stiffness and yield strength properties

Figure 5.3 provides experimental values of specific stiffness plotted against the specific yield strength for each of the fully optimised 3D projected 4-polytope metamaterials. Also included in the figure, are experimental values for gyroids and for hexagonal honeycomb structures tested out-of-plane. The data points represent the arithmetic mean value of five experimental samples tested in tension with vertical and horizontal error bars showing the full ranges of experimental values for specific stiffness and specific yield strength, respectively. All of the samples were manufactured using the same 3D prototyping technique as discussed in Section 3.4.

The experimental results follow a similar trend to the predicted simulation results, with the 8-cell metamaterial exhibiting the highest specific stiffness (0.89 MNm/kg) out of the 3D projected 4-polytope metamaterials, followed by the 5, 16 and 24-cell
5.2. EXPERIMENTAL RESULTS

Figure 5.3: Specific properties plot comparing the experimental results of the 3D projected 4-polytope metamaterials with gyroid and honeycomb structures in tension.

structures, the arithmetic means of which were 0.46, 0.40 and 0.39 MNm/kg, respectively. This is in-line with the predictions made from the simulation results where the cells with highly distributed strain energy density were found to have a higher capacity for storing strain energy and hence an overall higher stiffness. Specific yield strength values for the 3D projected 4-polytope metamaterials follow a slightly different trend, with the 8-cell structure still exhibiting the highest value of specific strength (6.71 kNm/kg), but this is then followed by the 5-cell, 24-cell and then 16-cell structures, the arithmetic means of which were 4.60, 4.48 and 3.13 kNm/kg, respectively. The higher specific strength of the 24-cell metamaterial as compared to
the 16-cell structure, is presumably a result of the central alignment of the 24-cell metamaterial unit cells enabling a higher level of elastic energy absorption prior to failure and suggesting that the unique geometrical features in individual unit cells of these metamaterials play an important role in determining the load bearing to the point of yield. Moreover, as shown by the simulation results summarised in Figure 5.2, the elastic strain energy density is more localised in the 16-cell structure than it is in the 24-cell structure. In addition, it can be observed that all 3D projected 4-polytope metamaterials have higher specific stiffness and strength values than the gyroid structure. When compared to the hexagonal honeycomb loaded in the out-of-plane direction, we note that the arithmetic means for each 3D projected 4-polytope metamaterial type is lower in terms of specific stiffness, and that only the upper experimental range of the 8-cell structure overlaps with the arithmetic mean value of the honeycomb. Nevertheless, the 8-cell structure has the highest specific yield strength when compared to any of the six structures presented here, including that of the hexagonal honeycomb. Here, the mean value is 1.05% higher than that of the honeycomb. Similarly to the hexagonal honeycomb, the 8-cell has thin-walled features aligned along the direction of loading and hence such an arrangement contributes towards the high specific stiffness and high specific yield strength values. Moreover, the 8-cell structure was developed using an optimisation approach which implicitly reduces stress concentration points by adjusting geometrical features within the unit cell. The 8-cell structure unlike the honeycomb, has cubic symmetry (i.e. identical mechanical properties in three orthogonal axes). The honeycomb structure in comparison, is essentially a 2-dimensional structure that is extruded in the 3rd dimension, and which has high stiffness and strength in only the out-of-plane direction.

The experimental specific stiffness and specific yield strength results discussed in the preceding paragraph are also summarised in Tables 5.1 and 5.2, respectively. The tables provide the arithmetic means, experimental ranges, medians, standard deviations and coefficients of variance. Additionally, the experimental results are compared against the simulation outputs using percentage differences and Z-score (Z) values. As shown in Table 5.1, the simulated specific stiffness results are 0.87%, 13.24%, 13.77% and 14.07% higher than the results obtained experimentally for the 8, 16, 5 and 24-cell structures, respectively. The Z-score values follow a similar trend and are between 0.20 and 9.12, with the 8-cell having the lowest Z-score, while the
5.2. EXPERIMENTAL RESULTS

16-cell has the highest. The results summarised here indicate that the simulation predicts the specific stiffness of the 8-cell structure with a good level of accuracy.

Table 5.1: Mean specific stiffness $\left( \frac{E}{\rho} \right)$ results for experimental 4-polytope-based metamaterial samples (5, 8, 16 and 24-cell) together with gyroid and hexagonal honeycomb results. The experimental results are compared against the simulated specific stiffness $\left( \frac{E}{\rho} \right)$ outputs using percentage differences and Z-score values.

<table>
<thead>
<tr>
<th>Experimental</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean specific stiffness $\left( \frac{E}{\rho} \right)$ (MNm/kg)</td>
<td>0.47</td>
<td>0.89</td>
<td>0.40</td>
<td>0.39</td>
<td>0.25</td>
<td>0.94</td>
</tr>
<tr>
<td>Upper value</td>
<td>0.50</td>
<td>0.95</td>
<td>0.41</td>
<td>0.47</td>
<td>0.28</td>
<td>0.98</td>
</tr>
<tr>
<td>Lower value</td>
<td>0.45</td>
<td>0.84</td>
<td>0.39</td>
<td>0.33</td>
<td>0.23</td>
<td>0.89</td>
</tr>
<tr>
<td>Median</td>
<td>0.47</td>
<td>0.87</td>
<td>0.41</td>
<td>0.37</td>
<td>0.24</td>
<td>0.96</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.019</td>
<td>0.038</td>
<td>0.007</td>
<td>0.053</td>
<td>0.020</td>
<td>0.033</td>
</tr>
<tr>
<td>CoV</td>
<td>4.12%</td>
<td>4.29%</td>
<td>1.67%</td>
<td>13.39%</td>
<td>8.18%</td>
<td>3.50%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific stiffness $\left( \frac{E}{\rho} \right)$ (MNm/kg)</td>
<td>0.55</td>
<td>0.90</td>
<td>0.47</td>
<td>0.46</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Percentage diff.</td>
<td>13.77%</td>
<td>0.87%</td>
<td>13.24%</td>
<td>14.07%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Z-score ($Z = \frac{\frac{E}{\rho} - \frac{E}{\rho}_{sim}}{S}$)</td>
<td>3.88</td>
<td>0.20</td>
<td>9.12</td>
<td>1.22</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

A different trend is observed when comparing specific yield strength results. The simulation output suggests higher values are possible, with the percentage difference ranging between 32.26% and 35.33%, while the Z-score values are between 3.63 and 11.42. This difference in simulation-predicted and experimentally tested behaviors can also be observed in Figure 5.4. Here, axial stress-strain curves obtained from simulations are plotted in dashed lines while the upper and lower experimental testing bounds are shown in solid lines. The simulations predict the sample stiffness with high accuracy, especially at low strain values and in each of the 3D projected 4-polytope metamaterials, the simulation results lie closer to the upper bound of the experimental results. As the tensile strain values increase, the gradients of the simulation and experimental curves start diverging indicating that the unit cell structures undergo plastic deformation at lower strain values than predicted by the compu-
5.2. EXPERIMENTAL RESULTS

Table 5.2: Mean specific yield strength \( \left( \frac{\sigma_y}{\rho} \right) \) results for experimental 4-polytope-based metamaterial samples (5, 8, 16 and 24-cell) together with gyroid and hexagonal honeycomb results. The experimental results are compared against simulated specific yield strength \( \left( \frac{\sigma_y}{\rho} \right) \) outputs using percentage differences and Z-score values.

<table>
<thead>
<tr>
<th>Experimental</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean specific yield strength ( \left( \frac{\sigma_y}{\rho} \right) ), (kNm/kg)</td>
<td>4.60</td>
<td>6.71</td>
<td>3.13</td>
<td>4.48</td>
<td>2.20</td>
<td>6.64</td>
</tr>
<tr>
<td>Upper value</td>
<td>4.91</td>
<td>7.13</td>
<td>3.31</td>
<td>5.29</td>
<td>2.34</td>
<td>6.83</td>
</tr>
<tr>
<td>Lower value</td>
<td>4.38</td>
<td>6.07</td>
<td>2.92</td>
<td>3.66</td>
<td>2.15</td>
<td>6.36</td>
</tr>
<tr>
<td>Median</td>
<td>4.56</td>
<td>6.74</td>
<td>3.17</td>
<td>4.34</td>
<td>2.17</td>
<td>6.74</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.202</td>
<td>0.354</td>
<td>0.161</td>
<td>0.588</td>
<td>0.072</td>
<td>0.192</td>
</tr>
<tr>
<td>CoV</td>
<td>4.39%</td>
<td>5.28%</td>
<td>5.15%</td>
<td>13.12%</td>
<td>3.29%</td>
<td>2.89%</td>
</tr>
</tbody>
</table>

Simulation

<table>
<thead>
<tr>
<th>Specific yield strength ( \left( \frac{\sigma_y}{\rho} \right) ), (kNm/kg)</th>
<th>6.91</th>
<th>10.37</th>
<th>4.81</th>
<th>6.62</th>
<th>N/A</th>
<th>N/A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percentage diff. (sim. vs exp.)</td>
<td>33.39%</td>
<td>35.33%</td>
<td>34.89%</td>
<td>32.26%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Z-score</td>
<td>11.42</td>
<td>10.35</td>
<td>10.40</td>
<td>3.63</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

The main reasons for such discrepancies are due to (1) manufacturing-related limitations and (2) a low number of neighbouring unit cells in the tensile samples. As discussed in Section 3.4 of Chapter 3, the experimentally measured mass was found to be higher than that calculated from the CAD models used in the simulations by 11.62%, 0.95%, 12.67% and 13.80% for the 5, 8, 16 and 24-cell structures, respectively. Higher mass directly affects the apparent density values leading to lower overall predictions of the specific properties when compared with simulation results. The 8-cell experimental samples were only 0.95% higher in mass than the equivalent CAD models while also having the most accurate simulated specific stiffness predictions with a difference of 0.87% between simulations and experiments. The structure with the highest noticeable difference between simulated and experimentally obtained specific stiffness results, the 24-cell (14.07%), also has the highest sample mass variation.
5.2. EXPERIMENTAL RESULTS

(13.80%). Higher sample mass can result from additional resin deposition within a unit cell during the manufacturing process. Any unwashed resin within the unit cell may accumulate at specific locations, such as corners and pockets. The additional resin partially cures during the post-curing process. This unwanted material may cause asymmetrical deformation of a structure under loading, giving rise to stress concentrations and leading to premature yielding.

This issue is further pronounced by the variations in material properties due to uneven polymer cross-linking during post-curing. As the samples are exposed to UV light, the level of polymerization is affected by the geometry of the metamaterial structure as well as its surface-to-volume ratio. As such, polymer cross-linking levels vary between individual samples as well as between different metamaterial sample sets. This variability can be observed in Figure 5.4 when comparing the upper and lower bounds of the experimental results.

In addition to these manufacturing-related limitations, the experimental results are affected by the low number of neighbouring unit cells in the tensile samples. The 2 × 2 unit cell arrangement in the cross-section of the tensile sample was chosen to ensure that the samples could be tested using the 32mm sized tensile testing grips, however, such an arrangement is far from ideal for a unit-cell-based metamaterial. In fact, simulation results by [166] suggest that the ideal ratio of sample cross-section to unit cell size should be higher than 10 to homogenise a mechanical metamaterial.

As the simulations do not account for manufacturing imperfections and have unit cell boundary conditions that are representative of an infinite-size sample, the simulation outputs compute an idealised metamaterial response. Thus, high prediction accuracy is observed for stiffness values at low strains while the stress levels within the structure are low, and geometrical as well as material property-related imperfections do not play a key role in the deformation of the metamaterial structure. As strain increases, the significance of the mentioned imperfections exacerbates causing the unit cell geometries to deform in an asymmetrical manner, therefore causing premature local point yielding of the structure. Consequently, this affects the observed experimental stress-strain behavior where the experimental samples tend to have a semi-linear part of the curve after the yield point which is different to the strain-softening type of behavior predicted by the simulations. Such behavior is believed to be a superposition of asymmetrical elastic deformation of the whole unit cell as well as the local point yielding within the structure due to sample imperfections.
5.2. EXPERIMENTAL RESULTS

Figure 5.4: Stress-strain plots for 5-cell, 8-cell, 16-cell and 24-cell 4-polytope-based metamaterials. Simulated results of axial stress along the direction of loading (S22) are presented as dashed lines while upper and lower experimental result bounds are shown as solid lines.
5.2. EXPERIMENTAL RESULTS

5.2.2 Effect of optimisation on other mechanical properties

The specific stiffness and strength results presented so far were engineered using a computational approach which aimed to maximise the total stored elastic strain energy in each of the 3D projected 4-polytope metamaterials. However, recognising how such an approach affects other mechanical properties allows us to compare 3D projected 4-polytope metamaterials in more detail, and to better understand the mechanical performance of these structures. Table 5.3 summarises the mean Young’s modulus, yield and tensile strengths, and modulus of resilience and toughness values for each of the 3D projected 4-polytope metamaterials, as well as for the gyroid and hexagonal honeycomb structures. The standard deviation (SD) and coefficient of variance (CoV) values are also included in Table 5.3 for each sample.

Table 5.3: Summary of experimentally obtained mechanical properties for 4-polytope-based metamaterials as well as gyroid and hexagonal honeycomb samples. The table presents Young’s modulus, yield and tensile strength and modulus of resilience and toughness values.

<table>
<thead>
<tr>
<th></th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, (MPa)</td>
<td>86.99</td>
<td>213.93</td>
<td>60.41</td>
<td>25.13</td>
<td>27.12</td>
<td>181.88</td>
</tr>
<tr>
<td>SD</td>
<td>3.58</td>
<td>9.18</td>
<td>1.01</td>
<td>3.37</td>
<td>2.22</td>
<td>6.36</td>
</tr>
<tr>
<td>CoV</td>
<td>4.12%</td>
<td>4.29%</td>
<td>1.67%</td>
<td>13.39%</td>
<td>8.18%</td>
<td>3.50%</td>
</tr>
<tr>
<td>Yield strength, (MPa)</td>
<td>0.85</td>
<td>1.62</td>
<td>0.47</td>
<td>0.28</td>
<td>0.24</td>
<td>1.28</td>
</tr>
<tr>
<td>SD</td>
<td>0.04</td>
<td>0.09</td>
<td>0.02</td>
<td>0.04</td>
<td>0.01</td>
<td>0.04</td>
</tr>
<tr>
<td>CoV</td>
<td>4.39%</td>
<td>5.28%</td>
<td>5.15%</td>
<td>13.12%</td>
<td>3.29%</td>
<td>2.89%</td>
</tr>
<tr>
<td>Tensile strength, (MPa)</td>
<td>1.44</td>
<td>3.67</td>
<td>1.24</td>
<td>0.65</td>
<td>0.97</td>
<td>2.08</td>
</tr>
<tr>
<td>SD</td>
<td>0.18</td>
<td>1.10</td>
<td>0.26</td>
<td>0.08</td>
<td>0.07</td>
<td>0.79</td>
</tr>
<tr>
<td>CoV</td>
<td>12.56%</td>
<td>30.12%</td>
<td>21.33%</td>
<td>11.98%</td>
<td>7.71%</td>
<td>38.02%</td>
</tr>
<tr>
<td>Modulus of resilience, (kJ/m³)</td>
<td>4.29</td>
<td>5.30</td>
<td>1.81</td>
<td>1.84</td>
<td>0.96</td>
<td>4.67</td>
</tr>
<tr>
<td>SD</td>
<td>0.30</td>
<td>0.52</td>
<td>0.13</td>
<td>0.23</td>
<td>0.06</td>
<td>0.40</td>
</tr>
<tr>
<td>CoV</td>
<td>7.06%</td>
<td>9.86%</td>
<td>7.10%</td>
<td>12.65%</td>
<td>6.10%</td>
<td>8.47%</td>
</tr>
<tr>
<td>Modulus of toughness, (kJ/m³)</td>
<td>14.06</td>
<td>44.12</td>
<td>15.63</td>
<td>11.56</td>
<td>25.88</td>
<td>17.45</td>
</tr>
<tr>
<td>SD</td>
<td>3.74</td>
<td>20.87</td>
<td>7.11</td>
<td>1.67</td>
<td>9.43</td>
<td>14.09</td>
</tr>
<tr>
<td>CoV</td>
<td>26.64%</td>
<td>47.30%</td>
<td>45.49%</td>
<td>14.48%</td>
<td>36.43%</td>
<td>80.75%</td>
</tr>
</tbody>
</table>
5.2. EXPERIMENTAL RESULTS

Table 5.4: Apparent and relative densities for simulated and experimentally tested samples. The table includes percentage difference values between simulated and experimentally obtained apparent densities.

<table>
<thead>
<tr>
<th></th>
<th>Simulations</th>
<th></th>
<th>Experimental</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apparent</td>
<td>Relative</td>
<td>Apparent</td>
<td>Relative</td>
</tr>
<tr>
<td></td>
<td>density, (kg/m$^3$)</td>
<td>density</td>
<td>density</td>
<td>density</td>
</tr>
<tr>
<td>5-cell</td>
<td>164.57</td>
<td>14.13%</td>
<td>183.70</td>
<td>15.77%</td>
</tr>
<tr>
<td>8-cell</td>
<td>238.81</td>
<td>20.50%</td>
<td>241.08</td>
<td>20.69%</td>
</tr>
<tr>
<td>16-cell</td>
<td>132.86</td>
<td>11.41%</td>
<td>149.70</td>
<td>12.85%</td>
</tr>
<tr>
<td>24-cell</td>
<td>55.78</td>
<td>4.79%</td>
<td>63.48</td>
<td>5.45%</td>
</tr>
<tr>
<td>Gyroid</td>
<td>N/A</td>
<td>N/A</td>
<td>108.82</td>
<td>9.34%</td>
</tr>
<tr>
<td>Hex honeycomb</td>
<td>N/A</td>
<td>N/A</td>
<td>192.89</td>
<td>16.56%</td>
</tr>
</tbody>
</table>

Stress-strain plots representative of the experimental results are summarised in Table 5.3 to provide a better insight into the experimental results. The 8-cell structure has the highest Young’s modulus of 213.93 MPa which is 17.62% higher than that of the hexagonal honeycomb structure tested in the out-of-plane direction with the value of 181.88 MPa. The 5-cell and 16-cell structures have values of 86.99 and 60.41 MPa, respectively, surpassing the gyroid which has Young’s modulus of 27.12 MPa. The structure with the lowest value of 25.13 MPa is the 24-cell, however, the 24-cell also has the lowest apparent density of 63.48 kg/m$^3$ out of the six experimentally tested samples as presented in Table 5.4. The coefficient of variance values for all of the samples are between 1.67% and 13.39% showing a high level of consistency between the experimental sample results.

A similar trend is observed when analysing yield and tensile strength results. The 8-cell structure has the highest values of 1.62 and 3.67 MPa for yield and tensile strength, respectively, which are 26.56% and 76.44% higher than those of the hexagonal honeycomb with 1.28 and 2.08 MPa for the yield and tensile strength results, respectively. Following the 8-cell and the hexagonal honeycomb, the highest yield strength values in descending order were obtained for 5-cell, 16-cell, 24-cell and gyroid structures, respectively. The tensile strength results follow a similar trend to those for yield. Following the 8-cell and hexagonal honeycomb structures, the highest tensile strength values, in descending order, were obtained for the 5-cell, 16-cell, gyroid and 24-cell structures, respectively. Although the trend is similar, it should be noted that the 24-cell structure yields at 16.67% higher stress in comparison to the gyroid structure, however, it has a 32.99% lower tensile strength value. These
results are expected since the 3D projected 4-polytope metamaterials were designed using computational methods to maximise the elastic strain energy storage capacity, which directly correlates to the overall stiffness of the structure.

The ability to absorb elastic strain energy can also be evaluated by comparing the modulus of resilience values for the experimental samples. The experimental results suggest that the 8-cell structure has the highest modulus (mean value) followed by the hexagonal honeycomb and then the 5-cell, with mean values of 5.30, 4.67 and 4.29 kJ/m$^3$, respectively. When expressed as a percentage difference with respect to the honeycomb value, the 8-cell has a 13.49% higher, while the 5-cell has an 8.14% lower modulus of resilience, suggesting that both the 8-cell and 5-cell metamaterials are highly suited for applications where elastic energy absorption is desirable. Both the 16-cell and 24-cell structures outperform the gyroid by 88.54% and 91.67%, respectively, in terms of the modulus of resilience. Lastly, as the tensile strain increases and the plastic deformation range is reached, all of the 4-polytope-based metamaterials fail at the tensile strain range between 0.018 and 0.034, which is higher than that of the honeycomb, which has a strain to failure value of 0.014, and lower than the gyroid, which has a strain to failure value of 0.042, as shown in Figure 5.5. The modulus of toughness (mean value) is highest for the 8-cell with a value of 44.12 kJ/m$^3$, which is 70.48% greater than that of the gyroid. The relatively high toughness of the 8-cell is a consequence of the high Young’s and plasticity moduli, while the gyroid has the second highest toughness due to the sample failing at high strains, rather than due to it having a high modulus. The rest of the experimental samples have toughness values that are within the range of 11.56 and 17.45 kJ/m$^3$.

5.2.3 Performance comparison with existing mechanical metamaterials

To compare the performance of the 4-polytope-based metamaterials against other metamaterial structures, performance indices, namely normalised Young’s modulus ($E/E_0$), normalised strength ($\sigma/\sigma_y$) and tensile strength/Young’s modulus ($\sigma_t/E_0$), were plotted against the relative density of the structures in Figure 5.5 (a), (b) and Figure 5.6, respectively. Here, $E_0$ and $\sigma_y$ are Young’s modulus and yield strength of the constituent material. Figure 5.5 also includes the data for G shellular and P shellular structures tested axially in compression rather than tension presented in
Figure 5.5: Experimental results for 4-polytope-based metamaterials, gyroid and honeycomb samples compared against P and G shellular structures [12, 17]. The figure represents (a) normalised Young’s modulus ($E/E_0$) and (b) normalised strength ($\sigma/\sigma_y$) values plotted against relative sample density. G shellular results are only shown in (a), generalised performance indices for honeycombs, foams and natural materials are shown in (a) and (b). All the data for P and G shellular structures and generic performance indices for foams, honeycombs and natural materials were obtained using axial compressive rather than tensile testing. Dashed lines represent scaling laws that are shown for P and G shellular and honeycomb structures based on the methodology and data presented in [3] and [12] respectively.

The research publications by Akbari et al. [17] and Nguyen et al. [12]. Additionally, the plots are overlaid with the generic performance ranges of honeycombs in
5.2. EXPERIMENTAL RESULTS

Figure 5.6: Experimental results for 4-polytope-based metamaterials, gyroid and honeycomb samples showing tensile strength/Young’s modulus ($\sigma_t/E_0$) performance index plotted against relative sample density. The plot includes scaling law trendlines for each sample set.

compression (grey), foams (light blue) and natural materials (light red) using the data made available in [12]. Dashed lines represent scaling laws calculated using the methodology presented in [3]. In Figure 5.5 (a), the scaling law illustrates the equation $\frac{E}{E_0} = (\frac{\rho}{\rho_0})^n$, where $E$ is homogenised Young’s modulus of the sample, $E_0$ and $\rho_0$ are Young’s modulus and density of the constituent material, respectively, $\rho$ is density of the sample, and $n$ is a positive integer empirically found for each structure. The values for $n$ (Figure 5.5 (a)) are 1.36, 1.70 and 1.34 for G shellular, P shellular and honeycomb structures respectively. Similarly in Figure 5.5 (b), the dashed line crossing the honeycomb sample data point illustrates equation $\frac{\sigma_t}{\sigma_y} = (\frac{\rho}{\rho_0})^n$, where $\sigma$ is tensile yield strength of the sample, $\sigma_y$ and $\rho_0$ are tensile yield strength and density of the constituent material, respectively, $\rho$ is density of the sample, and the value for
5.2. EXPERIMENTAL RESULTS

As shown in Figure 5.5 (a), 3D projected 4-polytopes tend to have higher normalised Young's modulus values when compared against the P shellular structures with the datapoints for 5, 8, 16 and 24-cell structures all situated above the predicted P shellular performance, as illustrated by the purple dashed line spanning across the full range of relative densities. When compared against the G shellular structures, also referred to as Gyroids and indicated in this figure by the yellow dashed line, all 3D projected 4-polytopes (with the exception of the 24-cell) exhibit higher normalised Young’s modulus values than are observed for G shellular structures. It can be noted that in general, the 4-polytope-based structures tend to lie closer to the generic honeycomb range with 5, 8 and 16-cell having relative densities in the range of 12.85% to 20.69% while the relative density of the 24-cell is 5.45%. The overall best-performing structure is the 8-cell, showing the highest values of normalised Young’s modulus.

Figure 5.5 (b) summarises the performance in terms of normalised strength for the 3D projected 4-polytope metamaterials, gyroid structures, and honeycomb structures tested in tension, and for P shellular [12] structures tested in compression. Similarly to the plot shown in (a), Figure 5.5 (b) also includes the generic performance ranges for honeycombs in compression, foams and natural materials. Since there can be significant observable differences between the strengths of mechanical metamaterials in compression and tension, we do not include P shellular or G shellular in compression in this plot. This is evidenced in Figure 5.5 (b) by the noticeable differences between honeycombs in compression and those tested in tension, a scaling law is shown by a dotted dark blue line to represent the honeycomb in tension. A point of note here, is that 8-cell and 16-cell structures in tension lie on the scaling law line for honeycomb in tension, in terms of both strength and relative density. However, the 24-cell and gyroid in tension lie above the line, indicating that when compared against their relative densities, these structures are stronger in tension than honeycombs, and 8-cell, 16-cell and 5-cell 3D projected 4-polytopes.

Figure 5.6 shows the tensile strength normalised by Young’s modulus of fully cured 3D printing resin, and is plotted against the relative density of the experimental samples summarised in Table 5.4. This normalization approach allows for the visualization of the strength gain due to the metamaterial structure, rather than its constituent material properties [164]. The structure with the highest tensile strength
5.3. **KEY FINDINGS**

to modulus ratio is the 8-cell indicating that the tesseract arrangement is highly effective for applications requiring high tensile stiffness and strength, as previously shown using stiffness and tensile strength values (cf. Table 5.3). In a descending order of performance, the 8-cell is followed by the hexagonal honeycomb, the 5-cell, 16-cell and gyroid structures with the 24-cell having the lowest strength gain as a result of its architecture. The figure also includes trendlines showing scaling laws calculated using the methodology presented in [3], \( \frac{\sigma_t}{E_0} = \left( \frac{\rho}{\rho_0} \right)^n \), where \( \sigma_t \) is tensile yield strength, \( E_0 \) and \( \rho_0 \) are Young’s modulus and density of the constituent material, respectively, \( \rho \) is density of the sample, and \( n \) is a positive integer empirically found for each structure. The values for \( n \) are 3.92, 4.01, 3.61, 2.76, 3.22 and 3.83 for 5, 8, 16, 24-cell, gyroid and honeycomb, respectively.

### 5.3  Key findings

In this chapter, a tensile set of novel mechanical metamaterial structures was designed and optimised for use under tensile loading. Using 3D projected 4-polytopes as a base structure. It was shown that this new class of parametrically optimised cubically symmetrical mechanical metamaterials exhibit superior properties of specific stiffness and strength when compared to more conventional structures such as gyroids and honeycombs. While gyroids are also cubically symmetric, each of the four 3D projected 4-polytope metamaterials outperformed the gyroid in terms of both specific stiffness and specific yield strength. Under the optimisation framework, the specific stiffness properties of the initial 4-polytope-based structures were improved by 122%, 72%, 163% and 469% for 5-cell (pentatope), 8-cell (tesseract), 16-cell (orthoplex) and 24-cell (octaplex) metamaterials. However, not all 4-polytope-based structures yielded promising final properties. In addition to the gyroid, the experimental results were also benchmarked against the well-known and commonly used hexagonal honeycomb structure tested in the out-of-plane direction. The optimised 8-cell (tesseract) structure exhibited a higher specific yield strength than the honeycomb and a marginally lower average specific stiffness. The results demonstrate that by coupling evolutionary algorithm-based optimisation methods with parametric design, the mechanical performance of mechanical metamaterials can be enhanced without compromising mass. While the focus of this chapter was specific stiffness and strength properties under tensile loading conditions, the design and optimisation framework presented in
Chapter 3 can also be used to optimise for a range of other mechanical properties under different loading conditions. This will be demonstrated for the case of shear loading in Chapter 6.
Chapter 6

Properties of the shear metamaterial set

This chapter introduces and analyses a 4-polytope-based metamaterial set developed to exhibit high specific stiffness properties when loaded in shear. Similarly to compression and tension sets, the shear set of metamaterials was produced using the simulation, optimisation and manufacturing methodology discussed in Chapter 3. The simulation outputs are discussed at the beginning of the chapter with a focus on specific shear stiffness properties while the experimental results conclude specific shear stiffness and shear yield strength values. In addition, the optimisation effect on other mechanical shear properties is discussed and the performance of the developed metamaterials is compared against the gyroid and honeycomb structures in shear. The shear strength gain due to geometrical feature arrangement rather than the bulk material properties is also compared and discussed in the second half of the chapter. The work presented in this chapter was published in [157]. Progressive optimisation outputs for shear metamaterial structures are presented in Figure B.3 of Appendix B while the full dataset is made available on the Edinburgh Data Share website [22].

6.1 Simulation results

The shear set of metamaterials was developed by employing the optimisation framework discussed in Section 3.2 of Chapter 3. The objective function aimed at maximising specific shear stiffness was used while the boundary conditions representative of a shear loading scenario were input to the finite element simulations. The unit cell designs were generated in an iterative manner and their performance was evaluated
6.1. SIMULATION RESULTS

and ranked according to the objective function. Figure 6.1 presents the results of the incremental performance advancement of each 4-polytope-based structure in the shear set. The stacked column chart shows the specific stiffness values of the metamaterials evaluated at several optimisation progression levels, namely at 0% (unoptimised), 25%, 50%, 75% and 100% of total optimisation (fully optimised) iterations.

![Specific shear stiffness comparison](image)

Figure 6.1: Specific shear stiffness comparison for the 5, 8, 16 and 24-cell polytopes in shear as the optimisation advances from unoptimised (0%) to fully-optimised (100%) state in 25% progression increments.

The incremental specific shear stiffness improvements shown here, represent the design space exploration carried out by the optimisation algorithm with higher performance enhancements during the intermediate iterations (optimisation levels 25%-75%) and smaller improvements as the near-optimum solution (fully optimised) is being approached. The specific stiffness improvements between the unoptimised and fully optimised structures were found to be 4152%, 1280%, 275% and 282% for 5, 8, 16 and 24-cell structures respectively. The percentage improvement values are highly dependent on the performance of the initial (unoptimised) structure which was designed without any insight from computer simulations, nevertheless, the results demonstrate the capabilities and the significance of using the simulation-based optimisation approach. The lowest performance improvement observed for the 24-cell metamaterial illustrates an improvement which is 2.75 times higher than that of the original design which is highly significant when designing metamaterials aimed for a specific application, in this particular case, shear. The structure with the overall
6.1. SIMULATION RESULTS

best specific shear stiffness properties was found to be the 5-cell structure with a value of 64.46 kNm/kg at the end of the optimisation cycle. It is also the design that benefited the most from the optimisation framework out of the four metamaterial unit cells analysed here once again demonstrating the potential and need for an optimisation-powered design solution.

Figure 6.2: Colour maps for each of the 4-polytope-based structures with each column illustrating optimisation progression at a different level: (i) 0% (unoptimised), (ii) 25%, (iii) 50%, (iv) 75% and (v) 100% of total optimisation (fully-optimised) metamaterial unit cells. The colour legend represents a range of elastic strain energy density (ESEDEN) values in J/cm$^3$ when the cells are loaded in shear to 0.10 strain.

Figure 6.2 presents the elastic strain energy density distribution (ESEDEN) for the 4-polytope-based unit cells at each of the incremental optimisation levels starting from 0% (unoptimised) to 100% (fully optimised) in 25% increments. The colour maps of each unit cell, namely 5, 8, 16 and 24-cell indicate the geometric regions that contribute the most towards bearing the shear loading and also providing the overall stiffness to the unit cell structure. The strain energy density is seen to be
more evenly distributed within the solid continuum of a structure as the optimisation progresses. As a result, more geometrically optimised structures, have an increased overall capacity in storing the elastic strain energy which in turn is related to the overall stiffness of a unit cell. Consequently, when the apparent density of the unit cells is factored in, the fully optimised unit cells have the highest specific shear stiffness values as previously illustrated in Figure 6.1.

Due to the direction and the nature of the applied shear loading (discussed in Section 3.2.3 of Chapter 3), it can also be seen that the geometrical features at the corners of each unit cell are the regions with higher strain energy density distribution and hence have a significant contribution towards the overall stiffness of a metamaterial, as can be seen in the right column of Figure 6.1 representing fully optimised unit cell structures. This can particularly be seen in 5-cell and 16-cell structures which also benefit from the internal unit cell geometrical features acting as cross-bracing and joining the corners of the unit cell. The internal geometrical features contribute towards sharing the strain energy within the unit cell, provide additional stiffness to the structure and therefore are the critical factors to 5-cell and 16-cell having the highest specific shear properties. Between the two mentioned structures, the strain energy is more evenly distributed within the 5-cell while the 16-cell has comparatively higher strain energy density concentration at the unit cell corners but lower strain energy density values within the internal cross-bracing structure resulting in lower overall strain energy storage capacity.

On the other hand, the 8-cell structure has a comparatively even distribution of the strain energy density within the structure, however, its geometry does not contain any cross-bracing geometrical features within the unit cell and therefore has lower specific shear stiffness than the 5-cell and the 16-cell. Lastly, the 24-cell structure has a few strain energy concentration spots along some of the structure’s outer edges and also inner geometrical regions that do not contribute to the overall strain energy storage capacity. This is partially due to the 24-cell having higher levels of geometrical complexity in comparison to other projected 4-polytope-based metamaterials resulting in more slender edges and sharper corner features within the unit cell. Such an uneven arrangement results in the lowest specific shear stiffness values out of the four unit cell structures discussed here.
6.2 Experimental results

6.2.1 Specific shear stiffness and shear yield strength properties

Experimentally obtained specific shear stiffness and specific shear yield strength values are presented in Figure 6.3 for the shear set of the 3D projected 4-polytope-based structures. The plot marks the arithmetic mean value of each specific property based on five specimens \( n = 5 \) tested for each structure while the vertical and horizontal bars represent the total range of experimental values obtained for each property. For comparison purposes, the data for cubically symmetrical gyroid structure and hexagonal honeycomb structure tested in an out-of-plane direction are also included in the plot. Both of these structures were manufactured in the same manner as the projected 4-polytope metamaterial samples with the fabrication technique detailed in Section 3.4 of Chapter 3.

The experimental specific shear stiffness results presented in Figure 6.3 closely follow the simulation predictions (Figure 6.1) with the 5-cell geometry having the highest specific stiffness value of 57.55 kNm/kg and the percentage difference of 10.71% when compared to the simulation output. In descending order, the experimental specific shear stiffness values are 52.73, 43.52, 29.58 kNm/kg for the 16-cell, 8-cell and 24-cell structures respectively. The difference between the simulation and experimental results were found to be 6.54%, 0.97% and 10.93% for 16-cell, 8-cell and 24-cell structures respectively indicating high simulation accuracy levels.

As previously shown by the modelling results (Section 6.1), the metamaterial structures with 1) geometrical features acting as stiffeners at the corner of each unit cell and 2) cross-bracing geometries joining the opposite corners of a unit cell significantly contribute towards increasing the shear resistance. This is evident in 5-cell and 16-cell geometries which outperform the rest of the investigated structures when comparing both, experimental and simulation, results. The specific shear stiffness results are comparatively lower for the metamaterials with geometrical features that are less in line with the shear forces, namely 8-cell and 24-cell structures. This is in line with the simulation results summarised in Figure 6.2 demonstrating that the unit cell geometries with less evenly distributed strain energy density tend to have lower strain energy storage capacity and therefore lower overall stiffness values.
6.2. EXPERIMENTAL RESULTS

Figure 6.3: Specific shear properties plot for experimental 4-polytope-based metamaterial samples together with gyroid and honeycomb structures.

For comparison, the experimental results of gyroid and hexagonal honeycomb structures are also compared in Figure 6.3. Similarly to 8 and 24-cell unit cells, these structures also do not possess geometrical features that could act as cross-bracing or corner-stiffening elements and therefore the specific shear stiffness values are 30.02 and 22.82 kNm/kg for gyroid and honeycomb respectively. When compared to the best-performing 4-polytope-based structure, the 5-cell surpasses the gyroid and hexagonal
honeycomb structures by 1.9 and 2.5 times, respectively, in terms of specific shear stiffness.

In addition to high specific shear stiffness values, all of the 4-polytope-based metamaterials, namely 5, 8, 16 and 24-cell, also outperform the gyroid and hexagonal honeycomb structures in terms of specific shear yield strength. As shown in Figure 6.3, 8-cell has the highest specific shear yield strength, followed by the 5-cell, 16-cell and 24-cell geometries with the values of 2.03, 1.66, 1.18 and 0.98 kNm/kg respectively. The yield strength values for the gyroid and hexagonal honeycomb were found to be 0.46 and 0.84 kNm/kg respectively. The experimental values obtained for the 8-cell, the best-performing structure in terms of the specific shear yield strength, are 4.41 and 2.41 times higher than those of the gyroid and hexagonal honeycomb structures respectively. These results indicate that although the 8-cell has lower specific shear stiffness than the 5 and 16-cell structures, its cubical geometry with thin walls aligned along the diagonal directions of a unit cell offers great strength when loaded in shear. The lack of cross-bracing elements in the unit cell geometry affects the overall stiffness of the structure, however, the interconnected thin walls and a well-balanced selection of feature sizes minimising internal stress concentrations are the two factors most plausibly contributing towards the high specific shear yield strength of the unit cell.

All of the 4-polytope-based metamaterials developed and analysed in this work, benefit from the cubically symmetrical unit cells which have identical mechanical properties along their three orthogonal axes. This is unlike the honeycomb structures which show significantly better out-of-plane than in-plane mechanical stiffness and strength [116]. The results presented here demonstrate that 4-polytope-based metamaterials can not only outperform commercially available honeycomb structures but also other commonly researched metamaterials with cubically symmetric unit cells, such as gyroid structures.

The simulation and experimental results discussed in the preceding paragraphs are also presented in Tables 6.1 and 6.2 summarising specific shear stiffness and specific shear yield strength results respectively. Statistical analysis details such as experimental range, median, standard deviation and the coefficient of variance (CoV) are included for the experimental results. The tables also present a comparison between experimental and simulation results with percentage difference values quoted for each sample set and a Z-score ($Z$) value calculated as $Z = \frac{G - \overline{G}}{S}$ for the specific shear
6.2. EXPERIMENTAL RESULTS

Table 6.1: Mean specific shear stiffness \( \left( \frac{\bar{G}}{\rho} \right) \) results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures and specific shear stiffness values \( \left( \frac{\tau_y}{\rho} \right) \) for simulated models: 5, 8, 16 and 24-cell metamaterials.

<table>
<thead>
<tr>
<th>Experimental</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean shear specific stiffness ( \left( \frac{\bar{G}}{\rho} \right) ), (kNm/kg)</td>
<td>57.55</td>
<td>43.52</td>
<td>52.73</td>
<td>29.58</td>
<td>30.02</td>
<td>22.82</td>
</tr>
<tr>
<td>Upper value</td>
<td>65.05</td>
<td>51.24</td>
<td>63.32</td>
<td>34.71</td>
<td>32.15</td>
<td>27.13</td>
</tr>
<tr>
<td>Lower value</td>
<td>50.40</td>
<td>37.81</td>
<td>17.60</td>
<td>20.98</td>
<td>26.56</td>
<td>18.11</td>
</tr>
<tr>
<td>Median</td>
<td>56.78</td>
<td>41.40</td>
<td>46.54</td>
<td>25.58</td>
<td>30.02</td>
<td>23.13</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>5.66</td>
<td>5.36</td>
<td>16.07</td>
<td>5.50</td>
<td>2.14</td>
<td>2.86</td>
</tr>
<tr>
<td>CoV</td>
<td>9.83%</td>
<td>12.32%</td>
<td>30.47%</td>
<td>18.59%</td>
<td>7.13%</td>
<td>12.55%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific shear stiffness ( \left( \frac{\tau_y}{\rho} \right) ), (kNm/kg)</td>
<td>64.46</td>
</tr>
<tr>
<td>Percentage diff. (sim. vs exp.)</td>
<td>10.71%</td>
</tr>
<tr>
<td>Z-score</td>
<td>1.22</td>
</tr>
</tbody>
</table>

stiffness case and as \( Z = \frac{\tau_y - \bar{\tau}_y}{S} \) for the specific shear yield strength case, where \( S \) is the standard deviation of each sample set.

As presented in Table 6.1, the simulation results for specific shear stiffness are 0.97%, 6.54%, 10.71% and 10.93% higher than experimentally obtained values for the 16, 8, 5 and 24-cell structures. Similar tendencies between the simulation outputs and experimental results are demonstrated by the low Z-score values which are in the range of 0.03 to 1.22 for the specific shear stiffness results. While the modelling outputs tend to overestimate the metamaterial performance, these results indicate that the simulation accuracy for predicting the specific shear stiffness values are high and the simulation and experimental results are in good agreement. The specific shear stiffness values are most accurately predicted for the 16-cell structure.

However, a different trend is present when analysing specific shear yield strength results summarised in Table 6.2. The percentage difference values comparing simulation and experimental results are in the range of 10.85% and 36.34% with the most
6.2. EXPERIMENTAL RESULTS

Table 6.2: Mean specific shear yield strength \( \left( \frac{\tau_y}{\rho} \right) \) results for experimental samples: 5, 8, 16 and 24-cell metamaterials, as well as gyroid and honeycomb structures, and specific shear strength values \( \left( \frac{\tau_y}{\rho} \right) \) for simulated models: 5, 8, 16 and 24-cell metamaterials.

<table>
<thead>
<tr>
<th></th>
<th>Experimental</th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean specific shear</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>yield strength ( \left( \frac{\tau_y}{\rho} \right) )</td>
<td>1.66</td>
<td>2.03</td>
<td>1.18</td>
<td>0.98</td>
<td>0.46</td>
<td>0.84</td>
<td></td>
</tr>
<tr>
<td>Upper value</td>
<td>1.90</td>
<td>2.19</td>
<td>1.88</td>
<td>1.29</td>
<td>0.52</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>Lower value</td>
<td>1.46</td>
<td>1.70</td>
<td>1.10</td>
<td>0.70</td>
<td>0.41</td>
<td>0.66</td>
<td></td>
</tr>
<tr>
<td>Median</td>
<td>1.67</td>
<td>2.13</td>
<td>1.12</td>
<td>0.87</td>
<td>0.46</td>
<td>0.83</td>
<td></td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.15</td>
<td>0.18</td>
<td>0.30</td>
<td>0.20</td>
<td>0.04</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>CoV</td>
<td>9.34%</td>
<td>8.73%</td>
<td>25.41%</td>
<td>20.47%</td>
<td>8.72%</td>
<td>13.44%</td>
<td></td>
</tr>
</tbody>
</table>

|                      | Simulation   |        |        |         |         |        |               |
| Specific shear       |              |        |        |         |         |        |               |
| yield strength \( \left( \frac{\tau_y}{\rho} \right) \) | 1.86 | 2.90  | 1.77   | 1.54    | N/A     | N/A    |               |
| Percentage diff.     | 10.85%       | 29.90% | 33.18% | 36.34%  | N/A     | N/A    |               |
| Z-score              | 1.30         | 4.89   | 1.95   | 2.79    | N/A     | N/A    |               |

accurate prediction of the 5-cell performance and the least accurate outputs for the 24-cell. The Z-scores are also indicating higher levels of discrepancies with the values of 1.30, 1.95, 2.79 and 4.89 in increasing order for the 5, 16, 24 and 8-cell respectively.

The results are also visualised in Figure 6.4 with the simulation-predicted stress-strain curves plotted in dashed lines and the upper and lower experimental testing bounds presented in solid lines. The specific shear stiffness results are predicted with high accuracy, especially at low strain rates with the simulation results closely following the upper experimental stress-stain curves for each of the 4-polytope-based metamaterials. This trend is especially evident at the low shear strains with the stress-strain curves starting to diverge and the experimental samples reaching the onset of plasticity at lower shear strain values than predicted by modelling. As the result, the 4-polytope-based metamaterials enter the plastic deformation stage earlier and experimental specific shear yield strength are lower than predicted by the simulations.
Figure 6.4: Shear stress-strain curves for 5, 8, 16 and 24-cell metamaterials. Upper and lower experimental bounds are presented in solid lines while simulated results are shown as dashed lines.
The main reasons contributing the most towards the differences between the simulated and experimentally obtained specific shear yield strength results are 1) manufacturing limitations, 2) shear testing limitations and 3) a low number of neighbouring unit cells in the shear specimens. Firstly, the manufacturing limitations stem from the limitations of SLA 3D printing methodology and the aim to manufacture geometrically complex structures. As discussed in Section 3.4 of Chapter 3, the 4-polytope-based metamaterial unit cells contain geometrical pockets where the resin tends to accumulate during the 3D printing process and is not fully removed when the samples are post-processed. The leftover resin then solidifies during the post-curing process, alters the intended unit cell geometry and contributes to creating stress concentration points and leading to an early onset of plasticity. This also results in a higher sample weight which negatively affects the specific properties of experimentally tested metamaterials. Secondly, the limitations of a 2D DIC system used for measuring the strains in a 3-point bend test contribute to the inaccuracies of the experimental results. The 2D system neither captures the out-of-plane nor the internal unit cell deformations and therefore contributes to the measurement-related inaccuracies. Thirdly, the maximum size of the specimens is limited by the build volume of the 3D printer, the samples have a low number of neighbouring unit cells and therefore suffer from boundary effects which are not accounted for in the simulations. The $2 \times 2$ arrangement of the unit cells in a cross-section of a specimen is considered as low as for a unit-cell-based structure. Computational modelling work published by [166] suggests that the ideal specimen cross-section to unit size ratio should exceed 10 to homogenise mechanical metamaterial.

It should also be noted that the modelling work presented here does not account for any manufacturing-related imperfections, assume periodic boundary conditions and hence idealise metamaterial performance. Therefore, at low shear strains when the stress levels within the material are low and material imperfections are not the key factors affecting the metamaterial response and therefore the specific shear stiffness predictions are of high accuracy. However, as the shear strains increase, the importance of the aforementioned imperfections increases as well causing unsymmetrical deformation of the unit cells and thus initiating premature local point yielding within the structure. As a result, this also affects the stress-strain response after the onset of plasticity with the simulation results suggesting different performance in the plastic deformation region to the experimentally observed stress-strain behaviour.
6.2. EXPERIMENTAL RESULTS

6.2.2 Effect of optimisation on other mechanical properties

Table 6.3: Summary of experimentally obtained mechanical properties: shear modulus, shear yield strength and shear strength, modulus of resilience and modulus of toughness for 4-polytope-based metamaterials, and for gyroid and hexagonal honeycomb structures.

<table>
<thead>
<tr>
<th></th>
<th>5-cell</th>
<th>8-cell</th>
<th>16-cell</th>
<th>24-cell</th>
<th>Gyroid</th>
<th>Hex honeycomb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear m., (MPa)</td>
<td>3.58</td>
<td>4.00</td>
<td>2.69</td>
<td>2.95</td>
<td>4.31</td>
<td>4.09</td>
</tr>
<tr>
<td>SD</td>
<td>0.35</td>
<td>0.49</td>
<td>0.80</td>
<td>0.58</td>
<td>0.41</td>
<td>0.51</td>
</tr>
<tr>
<td>CoV</td>
<td>9.83%</td>
<td>12.32%</td>
<td>29.58%</td>
<td>19.74%</td>
<td>9.52%</td>
<td>12.55%</td>
</tr>
<tr>
<td>Shear yield strength, (MPa)</td>
<td>0.10</td>
<td>0.19</td>
<td>0.08</td>
<td>0.10</td>
<td>0.07</td>
<td>0.15</td>
</tr>
<tr>
<td>SD</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>CoV</td>
<td>9.34%</td>
<td>8.38%</td>
<td>22.72%</td>
<td>21.69%</td>
<td>29.52%</td>
<td>13.44%</td>
</tr>
<tr>
<td>Shear strength, (MPa)</td>
<td>0.15</td>
<td>0.26</td>
<td>0.16</td>
<td>0.17</td>
<td>0.27</td>
<td>0.37</td>
</tr>
<tr>
<td>SD</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
<td>0.05</td>
<td>0.10</td>
</tr>
<tr>
<td>CoV</td>
<td>14.14%</td>
<td>11.42%</td>
<td>22.42%</td>
<td>18.59%</td>
<td>16.62%</td>
<td>26.12%</td>
</tr>
<tr>
<td>M. of resilience, (kJ/m³)</td>
<td>1754</td>
<td>4197</td>
<td>918</td>
<td>2260</td>
<td>649</td>
<td>2502</td>
</tr>
<tr>
<td>SD</td>
<td>164</td>
<td>606</td>
<td>179</td>
<td>373</td>
<td>126</td>
<td>335</td>
</tr>
<tr>
<td>CoV</td>
<td>9.34%</td>
<td>14.45%</td>
<td>19.54%</td>
<td>16.49%</td>
<td>19.47%</td>
<td>13.39%</td>
</tr>
<tr>
<td>M. of toughness, (kJ/m³)</td>
<td>24406</td>
<td>16840</td>
<td>15471</td>
<td>7215</td>
<td>34200</td>
<td>22965</td>
</tr>
<tr>
<td>SD</td>
<td>13318</td>
<td>4826</td>
<td>9110</td>
<td>2742</td>
<td>15470</td>
<td>8990</td>
</tr>
<tr>
<td>CoV</td>
<td>54.57%</td>
<td>28.66%</td>
<td>58.89%</td>
<td>38.00%</td>
<td>45.23%</td>
<td>39.14%</td>
</tr>
</tbody>
</table>

The mechanical metamaterial properties discussed up until now were highly influenced by the computational methods aimed at maximising the elastic strain energy capacity within the unit cell. This enabled the enhancement of specific shear stiffness and specific shear yield strength properties of the 4-polytope-based structures. However, to better understand the effect of the computational optimisation approach on other mechanical properties and hence the behaviour of these structures, Table 6.3 summarises shear modulus, shear yield and shear strength as well as modulus of resilience and toughness properties to evaluate metamaterial performance in a more generic sense. The values are presented for all of the 4-polytope-based metamaterials, gyroid and hexagonal honeycomb structures, the summary also includes statistical values for standard deviation (SD) and coefficient of variance (CoV).

The gyroid structure exhibits the highest shear stiffness with a modulus value of
4.31 MPa, closely followed by hexagonal honeycomb and 8-cell metamaterial structures which have a modulus value of 4.09 and 4.00 MPa respectively. The shear stiffness values for 5, 16 and 24-cell are 3.58, 2.69 and 2.95 MPa respectively. The coefficient of variance was found to be between 9.52% and 29.58% with standard deviation values between 0.35 and 0.80.

A different trend is seen when comparing the shear yield strength properties with the 8-cell structure having the highest value of 0.19 MPa which is 23.53% higher than that of a hexagonal honeycomb which is the second best-performing structure. The rest of the 4-polytope-based structures, namely the 5, 16 and 24-cell outperform the gyroid by 35.29%, 13.33% and 35.21% respectively which has the lowest stiffness among the compared metamaterials of 0.07 MPa. In terms of shear strength, the hexagonal honeycomb performs the best followed by the gyroid and the 8-cell with shear strength values of 0.37, 0.27 and 0.26 MPa respectively while the 5, 16 and 24-cell structures have the shear strength of 0.15, 0.16 and 0.17 MPa respectively.

The modulus of resilience results follow a similar trend as summarised for the shear yield strength with the 8-cell showing the maximum capacity for absorbing energy before the onset of plasticity outperforming both the gyroid and the honeycomb structures by 146.43% and 50.60% respectively. All of the rest 4-polytope-based metamaterials outperform the gyroid structure indicating the suitability of this new class of metamaterials for applications where the elastic energy storage in shear is of great importance.

The metamaterials with the highest modulus of toughness values, in descending order, are the gyroid, 5-cell and honeycomb with the modulus of toughness of 34200, 24406 and 22965 kJ/m$^3$ respectively. This is followed by the 8-cell, 16-cell and 24-cell structures with the respective modulus of toughness values of 16840, 15471 and 7215 kJ/m$^3$. Among the 4-polytope-based structures, the ones with the cross-bracing structural features, namely the 5 and 16-cell structures, tend to have a longer plastic region in comparison to 8 and 24-cell structures that lack the geometrical features joining the opposite corners of a unit cell together. The high modulus of toughness in 5-cell and 16-cell structures is mainly the result of the ability to sustain high shear strains prior to the occurrence of catastrophic failure with 5-cell and 16-cell failing at the shear strains of 0.13 and 0.10 respectively. This demonstrates the ability of the structures to absorb shear deformation energy through gradual plastic yielding, however, it is unclear how this behaviour occurring in only two of the four
6.2. EXPERIMENTAL RESULTS

investigated 4-polytope-based structures is affected by the parametric optimisation aimed at maximising elastic strain energy storage.

Table 6.4: Apparent and relative densities for simulated and experimentally tested shear samples.

<table>
<thead>
<tr>
<th></th>
<th>Simulations</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apparent density, (kg/m$^3$)</td>
<td>Relative density</td>
</tr>
<tr>
<td>5-cell</td>
<td>56.44</td>
<td>4.85%</td>
</tr>
<tr>
<td>8-cell</td>
<td>86.71</td>
<td>7.45%</td>
</tr>
<tr>
<td>16-cell</td>
<td>53.86</td>
<td>4.63%</td>
</tr>
<tr>
<td>24-cell</td>
<td>96.25</td>
<td>8.27%</td>
</tr>
<tr>
<td>Gyroid</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Honeycomb</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

The results presented here provide a good indication of the metamaterial performance, however, they do not take the mass of each specimen into account. Table 6.4 summarises the apparent and relative densities of the simulated and experimentally tested structures compared in this publication. It is worth noting that the gyroid and hexagonal honeycomb structures which have the highest shear stiffness and strength properties also have the highest apparent density values. When compared to the 4-polytope-based metamaterials, the apparent density values of gyroid and honeycomb specimens are 79.11% and 96.97% higher than the 5-cell and 43.75% and 64.30% higher than the 8-cell which has the highest apparent density out of the three best-performing 4-polytope-based metamaterials. This emphasises the importance of comparing metamaterial structures using specific properties when ranking their performance.

6.2.3 Performance comparison with existing mechanical metamaterials

An alternative way of comparing the structural performance of the metamaterials is presented in Figures 6.5 and 6.6. Here, the experimental results of 4-polytope-based metamaterials as well as gyroid and hexagonal honeycomb samples are compared using performance indices plotted against the relative density of each experimental sample. This normalisation method allows examining the stiffness and strength gained from the metamaterial structure rather than the bulk material properties [164].
6.2. EXPERIMENTAL RESULTS

Figure 6.5: Experimental comparison of 4-polytope-based metamaterials with gyroid, hexagonal honeycomb samples, as well as other metamaterial structures presented in, [18, 19], namely, Kelvin, octet, idealised foam and cubic lattices. The figure presents the results for (a) normalised shear modulus ($G/G_0$) and (b) normalised shear strength ($\tau/\tau_0$) plotted against the relative density. Parts (b) of the figure also include scaling law trendlines for all 4-polytope-based metamaterial structures and gyroid and hexagonal honeycomb samples.

Figure 6.5 (a) presents normalised shear modulus ($G/G_0$) with additional data included for metamaterial structures presented in, [18, 19], namely, Kelvin, octet, idealised foam and cubic lattices. It is evident that all 4-polytope-based metamaterials outperform idealised foam and cubic lattice structures in terms of normalised shear modulus at a given relative density. The 5-cell and 16-cell structures also perform
better in comparison to the Kelvin lattice structure while only the 5-cell structure has a similar normalised shear modulus to the octet truss.

In terms of normalised shear strength (Figure 6.5 (b)), 16-cell surpasses the rest of the 4-polytope-based metamaterials and is closely followed by the 5-cell structure both of which have similar geometrical cross-bracing features as discussed in Section 6.1. In the descending performance order, these two metamaterial structures are followed by the 8-cell, 24-cell, gyroid and hexagonal honeycomb structures.

The plot in 6.6, shows the shear yield strength normalised by the shear modulus of the fully cured constituent material while this is presented against the relative density of each structure (also shown in Table 6.4).

Figure 6.6: Shear yield strength over shear modulus ($\tau_y/G_0$) plotted against the relative density for experimental comparison of 4-polytope-based metamaterials with gyroid, hexagonal honeycomb samples. The figure includes scaling law trendlines for all 4-polytope-based metamaterial structures and gyroid and hexagonal honeycomb samples.
6.3 Key findings

This chapter presents the set of mechanical metamaterials optimised for shear resistance which was developed as a part of an emerging class of 4-polytope-based metamaterials. The use of methodology presented in Chapter 3, demonstrates that the performance of these structures can not only be tailored to a specific application...
6.3. **KEY FINDINGS**

but also enhanced more than 40 times in terms of specific shear properties by employing an evolutionary algorithm-powered optimisation framework. The simulation and experimental results suggest that cubically symmetrical 4-polytope-based metamaterials outperform other commonly researched structures such as gyroid and hexagonal honeycombs in terms of both specific shear stiffness and specific shear yield strength. Among the structure examined here, the 5-cell (pentatope) demonstrates a shear stiffness that is nearly double that of a gyroid structure. This superior performance is attributed to the presence of cross-bracing within the 5-cell which is also present in the second-best-performing 16-cell structure. The 8-cell (tesseract) shows the highest specific shear yield strength 2.4 times surpassing the hexagonal honeycomb tested in the out-of-plane direction and hence offering the advantages where a high strength-to-weight ratio is required. The 24-cell structure demonstrates the lowest values for both specific shear stiffness and shear yield strength out of the four investigated 4-polytope-based structures while having almost the same specific shear stiffness as the gyroid and higher specific shear yield strength than the hexagonal honeycomb. The normalised shear modulus results are also benchmarked against a range of metamaterial structures investigated in the available literature showing the potential of the 4-polytope-based metamaterials. The cubically symmetrical 4-polytope design, lightweightness and high shear resistance provide significant benefits in maintaining structural stiffness when subjected to multi-axial loading which is advantageous in many real-life applications within the transport and aerospace sector.
Chapter 7

Comparison and evaluation of the optimised metamaterial sets

This chapter builds on the results presented in Chapters 4, 5 and 6 and compares the developed metamaterial sets. It looks into the geometrical features within each unit cell design and considers their contribution towards the mechanical performance of 4-polytope-based metamaterials. The chapter also discusses the limitations of the work, including simulation, optimisation, manufacturing and mechanical testing associated limitations, and suggests unit cell design simplifications as a part of future work. Additionally, the potential applications and viability of this new class of metamaterials are discussed.

7.1 Comparison of the unit cell sets developed for compression, tension and shear

The final best-performing unit cell designs for each of the developed metamaterial sets are shown in Figure 7.1. The following paragraphs discuss the three optimised mechanical metamaterial sets in the following order; first, the compression set (shown in the top row of Figure 7.1 in grey) is evaluated which is followed by the tension set (shown in the middle row in blue) and lastly the shear set (bottom row in green).

Along with the parametric design variables (as previously presented in Table 3.2), this section also uses the inner and outer features of the geometries to describe and evaluate the features of the best performing structures. To aid the discussion, Figure 7.2 illustrates two sets of geometrical features, namely the inner features in light
7.1. COMPARISON OF THE UNIT CELL SETS DEVELOPED FOR COMPRESSION, TENSION AND SHEAR

Figure 7.1: Comparison of the best-performing unit cell structures in all three optimised metamaterial sets, namely, compression (in grey), tension (in blue) and shear (in green). The structures with the highest specific (axial/shear) stiffness values within each set are marked in dashed red while the ones with the highest specific (axial/shear) strength are marked in solid yellow.

First, as shown in the top row, the optimisation results for the compression set favour the unit cells with a more open geometrical arrangement where the outer walls are eroded exposing the inner geometry of the unit cell. The optimisation algorithm arranges the outer wall features to act as a frame-like structure with increased wall thickness but narrower features around the edges of the cell. This is especially prominent in 5-cell and 16-cell structures with narrow outer wall features with higher wall thickness. In the case of the 8-cell, the inner cube geometry is enlarged significantly to serve as the described frame-like structure. In fact, the 8-cell compression struc-
7.1. COMPARISON OF THE UNIT CELL SETS DEVELOPED FOR COMPRESSION, TENSION AND SHEAR

Figure 7.2: Illustration of inner and outer geometrical features within each 4-polytope-based unit cell.

ture has the inner cube size (parametric design variable D for 8-cell in Figure 3.2) which is 57.47% and 39.20% larger than the equivalent tension and shear structures respectively. The 24-cell structure also follows a similar geometrical trend having the largest diameter drain holes (previously discussed in Section 3.1.1 of Chapter 3). This is another way for the algorithm to erode the outer unit cell walls with the compression structure having the drain holes (parametric design variable B for 24-cell in Figure 3.2) which are 88.24% and 41.18% larger in comparison to the equivalent structures developed for tension and shear respectively. This optimisation output results from the need to reduce the number of possible instances where buckling can occur within the unit cell structures as long thin-walled features are prone to deform in this manner under compressive loads.

Second, the tension set in the middle row of Figure 7.1 is examined in more detail where the general trend in these structures is in favour of wider outer wall features of the unit cells with decreased wall thickness. This is observed when comparing the outer shell round features (parametric design variable J for 5-cell and F for 16-cell in Figure 3.2) which contribute to the wide outer walls of the unit cell. In the case of the 16-cell tension structure, this feature is 6.01 and 1.72 times larger when compared to the equivalent compression and shear structures respectively. The drain holes have a smaller diameter when compared to both the compression and the shear sets which as a result creates wider thin-walled features. To be specific, the drain hole sizes in all 4-polytope-based tension set unit cells are on average 28.06% and 35.57% smaller than for compressive and shear structures respectively. Similarly, the inner geometrical features within the unit cell favour wider thin-walled structures rather
than narrower thicker walls. This is observed when comparing with the compression set equivalent 5-cell, 16-cell and 24-cell structures. In the case of the best-performing 8-cell structure, the inner cube size is the smallest out of the three presented sets making the outer walls of the unit cell longer. The 24-cell structure also demonstrates small diameter drain holes and wider internal geometrical features which is in line with the thin-walled trend among the structures in the tension set.

Although the compression and tension sets are both developed considering different types of axial loading, as the buckling effect is irrelevant in the tensile loading scenario, the optimisation yields thin-walled and wide-featured rather than thick-walled and narrow-featured unit cell features. Regardless of this fact, the best-performing unit cells in terms of specific stiffness and specific strength in both compression and tension sets are the 8-cell structures. This is attributed to the fundamental geometrical properties inherited from the 3D projection of the 4D dimensional 8-cell structure. Both of the discussed 8-cell structures, optimised for compression and for tension, have most of the geometrical features aligned along the direction of the axial loading which act as load-carrying members and hence contribute to the superior performance of the unit cells.

Lastly, the shear set of 4-polytope-based unit cells demonstrates another different arrangement of geometrical features most optimal for the performance under shear loading. As shown in Figure 7.1, the more open unit cell arrangement with the walls being eroded is prominent. Similar to the structures presented in the compression set, the drain hole diameters are large, the outer walls form frame-like structures around the edges of the unit cell and the inner features in the 5-cell and 16-cell structures are thick-walled and narrow-featured rather than thin-walled and wide-featured. In the case of the 8-cell shear structure, the main drain hole (parametric design variable B for 8-cell in Figure 3.2) is 35.27% and 57.50% larger than within the equivalent compression and tension structures respectively, which completely erodes the inner cube feature within the unit cell. In addition, the importance of rounded corners and edges becomes evident in the shear set. This is best seen in the 5-cell and 16-cell structures (parametric design variable J for 5-cell and F for 16-cell in Figure 3.2) with the corners of the triangular outer wall cuts being rounded to reduce stress concentrations and more evenly distribute the strain energy density (refer to Figure 6.2 in Chapter 6 for more detail) at the unit cell edges. Similarly, the rounded features are present around the edges of the 24-cell and the 8-cell (parametric design variable
7.2. LIMITATIONS AND MITIGATION STRATEGIES

D for 24-cell and G for 8-cell in Figure 3.2) at the locations where the inner geometry meets the outer walls of the structure.

The structure demonstrating the highest specific shear stiffness values within the shear set is the 5-cell which is attributed to the presence of the cross-bracing inner geometry of the cell. Similar features are also present in the second-best-performing 16-cell structure. The structure with the highest specific shear strength in this set is the 8-cell. It is worth emphasising that the most optimal arrangement for the structure does not have the inner cube geometry which is present in the compression and tension sets. Judging from the iterative optimisation results for the 8-cell structure, the additional thin walls parallel to the shear loading direction do not significantly contribute to the strength and stiffness of the structure and are therefore made obsolete in favour of mass reduction.

It should be noted that while the trends for parametric design variable arrangement (drain hole sizes, wall thicknesses, round radii, etc) favouring a particular loading condition were observed, the correlation between individual variables and the objective function was found to be weak. As a result, it is cumbersome to attribute a few variables to the superior performance of a structure and therefore formulate definitive design guidelines. The research presented and analysed here demonstrates that the superposition of all the variables dictates the suitability of a structure for a specific loading condition which strengthens the case for exploratory optimisation algorithm use in metamaterial design.

7.2 Limitations and mitigation strategies

This section focuses on discussing limitations related to the simulation, optimisation, manufacturing and mechanical testing of the developed metamaterials and the appropriate mitigation techniques that were employed in this work.

7.2.1 Simulation related limitations

As previously discussed in Sections 3.1 and 3.2 of Chapter 3, the development of 4-polytope-based metamaterials heavily relied on the finite element simulations guiding the unit cell designs. All constituent material parameters used in FE simulations were obtained experimentally by testing five cylinder-shaped samples as described in Section 3.2 of Chapter 3. Nevertheless, the FE simulation method itself has a
few limitations that are worth noting. Firstly, only the elasto-plastic models were
used to define the unit cell simulations which predicted the plastic deformation of the
structure till the fracture strain is reached and the simulation is terminated. This did
not affect the prediction of the specific (axial or shear) stiffness properties, for which
the simulation results are presented in Chapters 4, 5 and 6. But, at the same time, it
did not allow for an accurate prediction of specific (axial or shear) strength properties.
However, this is considered to be beyond the scope of this study as the optimisation
objectives for all three loading conditions focused on maximising specific stiffness
while the specific strength values were only presented as a part of the experimental
testing output.

Secondly, the simulations did not consider the viscous effects of the additively
manufactured material. Although the photoreactive thermosetting resin used for the
manufacturing of the samples shows a viscous response at low strain rates, its effects
become negligible after a certain strain rate is reached. Therefore, to mitigate this
modelling limitation, all of the experimental samples tested as a part of this work
were loaded at a ramp rate of 10 mm/min (strain rate of 0.011 s\(^{-1}\)), a rate at which
cured neat resin exhibits Hookean behaviour under deformation.

Thirdly, the models did not consider the 3D printing orientation of the manu-
factured samples, which in some cases may lead to lower material properties in the
direction (Z-axis direction) perpendicular to the cured layers of the material. This
was not considered in the simulations mainly due to the fact that specimens produced
using a low-force-sterolithography process have highly isotropic material properties
along the orthogonal directions of a sample. In fact, the experimental data obtained
specifically for the fabrication method employed in this work shows that the variation
in tensile and compressive Young’s moduli in the Z-axis direction compared to the
other two orthogonal directions is less than 4.25% and 5.73% respectively. Similarly,
the variation in the tensile and compressive strength values was found to be less than
5.02% and 6.13% respectively. These findings are in line with the results published
on a fabrication method using the LFS technique presented in [167]. As the quoted
variations in material properties due to the orientation sample orientation are below
the 10% mark, further improvements of the modelling approach in this area were
deemed out of the scope of this work.
7.2.2 Optimisation related limitations

A few limitations and mitigation approaches relevant to the optimisation framework development for this work should be noted. It is built on the aforementioned simulations and relies on GA to search for the best-performing geometrical unit cell arrangements. The algorithm has its limitations in finding the best solution due to its meta-heuristic nature. In other words, this search method yields near-optimum solutions rather than finding the global best solution due to its limited knowledge of the design space. This is closely linked to the ability of genetic algorithms to perform optimisation in the design spaces, such as the optimisation problem solved in this study, by making minimal assumptions about the optimisation problem at hand. The approach where no problem-specific knowledge is provided to the optimisation framework is beneficial in avoiding inherent human biases influencing the final solution of the problem. The chosen approach for mitigating the limitation was to ensure that the algorithm can explore a wide range of possible solutions prior to reaching the predefined termination condition. This was implemented by setting the absolute number of generations parameter to an infinite value and instead introducing a stopping criterion which terminates the search once the results show no significant improvement (less than 5% improvement) over the next 20% of the total generation number from the best (near optimum) solution. This K-iterations termination criterion was formulated based on the research presented in [168, 169, 170]. Although such an approach might be considered computationally inefficient, with a fifth of total simulations having no practical value to final solutions, it offers a significantly increased reliability of the search results.

7.2.3 Manufacturing associated limitations

The 3D printing bay size was identified as one of the key limiting factors for the number of stacked unit cells that could be printed in a single metamaterial sample. In the case of manufacturing tension and shear specimen sets (see Figure 7.3 (b) and (c)), the Form 3 3D printer platform size acted as the determining factor limiting the external sample length ($L$) to 120 mm. Together with some mechanical testing related limitations further discussed in Section 7.2.4 of this chapter, the final external sample dimensions were constrained to $30 \times 30 \times 120$mm ($B \times H \times L$). This resulted in metamaterial arrays that have $2 \times 2 \times 4$ arrangement with 16 unit cells in total.
for the tension specimen set and $2 \times 2 \times 8$ arrangement with a total of 32 unit cells for the shear specimen set. The sample set with only 2 unit cells across the breadth ($B$) and height ($H$) of a specimen yields reliable experimental results but is not ideal for fully capturing the potential of newly developed metamaterials. As previously discussed in Section 5.2.1 and Section 6.2.1 of Chapters 5 and 6 respectively, the ideal specimen cross-section to unit size ratio should 10 or higher to homogenise a mechanical metamaterial, according to the work published in [166]. However, the manufacturing of samples with larger dimensions, for tension and shear sets, was simply not possible considering the available 3D printing and also mechanical testing equipment.

The compression set of the samples was unaffected by this dimensional restriction as due to the cubic shape of the samples, a $5 \times 5 \times 5$ arrangement fitted on the printing platform. This was considered to be sufficient, based on the experimental approaches presented in similar metamaterial studies [4, 76].
resin once the 3D printing process is finished. As presented in Section 3.4 of Chapter 3, a post-processing procedure is then used to wash the specimens and removed the uncured resin. Section 3.1.1 of the same chapter also discussed introducing the drain holes to all of the 4-polytope-based unit cell designs to aid the process of washing the uncured resin. With these design changes introduced, the experimental results presented in Chapters 4, 5 and 6 still demonstrate that the perfect removal of the uncured resin is not possible even from openly exposed features of the unit cells and a certain amount of uncured resin is always present in the manufactured samples. One of the reasons for this is the fact that the resin located at the perimeter of each 3D printed layer does not fully cure when exposed to the laser light due to the boundary effects. The second reason is related to the geometrical complexity of the metamaterial structures and small geometrical features located within the internal pockets of the structure that tend to accumulate the resin.

To circumvent this problem, a unit cell geometry-specific washing procedure was developed for the metamaterial samples adjusting the isopropyl alcohol circulation speed within the washing bath, changing circulation direction and adjusting washing time. The isopropyl alcohol concentration was tracked using a hydrometer to ensure the solvent is replaced once the resin content reaches 10-12%, as recommended by the washing equipment manufacturer [171]. Additionally, the post-processing tasks were executed in batches to ensure that the washing quality is consistent between the specimens within the same testing set.

### 7.2.4 Mechanical testing associated limitations

In addition to the manufacturing-related limitations, the metamaterial sample size was also constrained by the testing equipment used for mechanical characterisation. The breadth ($B$) and height ($H$) of the tensile metamaterial set samples were chosen to ensure that they can be tested using the 32 mm sized tensile testing grips on the Instron 8802 servo-hydraulic test machine as described in Section 3.5.2 of Chapter 3. This, therefore, limited the metamaterial sample size in terms of breadth ($B$) and height ($H$) to 30mm, resulting in the final external sample dimensions of $30 \times 30 \times 120$ mm.

The physical size of the shear samples was constrained in a similar manner due to the width of a 3-point bend fixture (detailed in Section 3.5.3 of Chapter 3) which led to a $2 \times 2$ unit cell arrangement across the breadth ($B$) and height ($H$) of a shear
7.3 Design simplifications for future work

To overcome some of the existing design limitations and increase the economical viability of the developed metamaterials, the unit cell designs presented in Chapters 4, 5, 6 could be geometrically simplified. This is beyond the scope of the work presented here and should be explored in the future. As the structures shown in Figure 7.1 comprise a mixture of thick and narrow or thin and wide geometrical features (discussed in Section 7.1), the geometrical complexity of separate features could be reduced to sets of truss-like and plate-like features. The research presented in the aforementioned chapters identifies the main performance trends, benefits, key geometrical features and limitations of the unit cell designs developed for each loading application and therefore lays the groundwork for further development of this new class of mechanical metamaterials.

Reducing the geometrical complexity of the 4-polytope-based unit cell designs while building on the knowledge summarised in this work could not only yield the opportunity to increase the technology readiness level (TRL) but would also allow exploring new methods for (1) designing, (2) simulating and (3) manufacturing the developed metamaterials. From a unit cell design perspective, using truss-like and
plate-like geometrical features would enable the transition towards a simpler geometrical definition using vertices and edges of the 3D projected 4-polytope wireframes rather than solid CAD models. This would enable a full parametrisation of the structures and increase the robustness of parametrically adjustable unit cell designs. Such a change in the design approach, moving from solid models to plate and truss structures, is now feasible due to the key geometrical features contributing to the mechanical performance of the 4-polytope wireframes being identified in this work.

From a computational standpoint, simplifying the unit cell geometries would also significantly reduce the computational efforts by moving from three-dimensional (tetrahedral) mesh elements, employed in this work, to less computationally expensive one-dimensional (line or beam) elements representing truss-like features and two-dimensional (triangular or quadrilateral) elements representing plate-like features. This would offer a few orders of magnitude reduction in computational time and costs when compared to simulating and optimising designs represented using solid 3D mesh elements. For example, simulating the 5-cell structure optimised for compressive loading using beam rather than solid mesh elements cuts a single simulation time from approximately 19 minutes (1140 seconds) to 11 seconds, two orders of magnitude difference. This could open new computational design research avenues for developing surrogate models, replacing finite element simulations, based on several thousands of previously obtained simulation data points and therefore offering quick and accurate optimisation solutions. Shorter simulation and optimisation times could also allow for more in-depth exploration of functionally graded materials by varying the apparent density and geometrical arrangement of the developed unit cells within a single metamaterial array.

The design simplification would also aid the manufacturability of the metamaterials as less complex unit cells would not require such a high-accuracy fabrication process. The use of truss-like and plate-like lattices could potentially solve some additive manufacturing-related limitations (previously discussed in more detail in Section 7.2.3 of Chapter 3). Moreover, new manufacturing methods could be explored such as kirigami-based cutting and folding of flat sheets to produce plate and truss structures forming individual unit cells. A similar approach for kirigami folding of cubic and octet geometries [10], truncated octahedron [172] and several lattice types [173] have previously been shown feasible, just to mention a few, and has the potential to scale up the manufacturing of metamaterial arrays if robotic automation is used.
7.4. EMERGING APPLICATION AND CHALLENGES FOR MECHANICAL METAMATERIALS

All of the aforementioned suggestions on the unit cell design simplification could be pursued to further the development of 4-polytope-based metamaterials, increase the TRL level and aid their adoption in real-world applications. These design suggestions should build on the existing knowledge presented and the insight provided in this thesis.

7.4 Emerging application and challenges for mechanical metamaterials

According to a report published by Nasdaq OMX in late 2022 [174], the estimated worth of the metamaterial market was US$ 284.10 million with a prediction for compound annual growth rate (CAGR) of around 36.20% for the next 5 years. It is estimated that the market should hit US$ 1,813.57 million by 2028. The findings are in line with other similar market analyses and predictions for metamaterial sector development in the near future [175, 176] identifying aerospace, transport, energy and healthcare as the main sectors that could benefit from the development of mechanical metamaterials.

This quick growth of the industry is attributed to the unlocked potential of metamaterial technology and the potential benefits that these structures can offer due to advancements in AM technology and the increasing availability of computational resources. The summary of the strength, weaknesses, opportunities and threats (SWOT) analysis for the generic mechanical metamaterials is shown in Figure 7.4 while the specific applicability of these concepts to the 4-polytope-based metamaterials is further discussed in the paragraphs below.

The ability to artificially engineer unique properties, tailor the response in a selective manner and enhance the performance are just a few of the many strengths of mechanical metamaterials. Moreover, the flexibility in exploring the wide design space enables the creation and discovery of metamaterials that exhibit unconventional properties and offer multiple functionalities. The mentioned strengths apply to the 4-polytope-based metamaterials presented in this work as they were designed to possess unique properties and further tailored and optimised to enhance performance under specific loading conditions. The exploration of the design space using a genetic algorithm demonstrates the design flexibility which can be achieved by modifying the geometrical parameters of the unit cell while the simulation and experimental
7.4. EMERGING APPLICATION AND CHALLENGES FOR MECHANICAL METAMATERIALS

<table>
<thead>
<tr>
<th>4-polytope-based metamaterials</th>
<th>Strengths</th>
<th>Weaknesses</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• Unique properties</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Tailorability</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Performance enhancement</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Design flexibility</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Multifunctionality</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Higher TRL work</th>
<th>Opportunities</th>
<th>Threats</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• Industrial applications</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Advanced manufacturing</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Sustainable solutions</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Cost considerations</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Alternative technologies</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Standardization challenges</td>
<td></td>
</tr>
</tbody>
</table>

Figure 7.4: Strengths, weaknesses, opportunities and threats (SWOT) of mechanical metamaterials

Results presented in Chapters 4, 5 and 6 show the suitability for applications requiring high specific stiffness and strength at the same time. The combination of these reasons contributes to the superior 4-polytope-based metamaterial performance when compared to honeycomb and gyroid structures. To be specific, 5, 8 and 16-cell structures surpass the gyroid structures in terms of both specific stiffness and specific yield strength in all three of the investigated loading cases. Moreover, the respective best-performing 8-cell designs, within the compressive and tensile metamaterial sets, outperform the hexagonal honeycomb structure by 17.34% and 1.05% respectively in terms of specific yield strength and in the case of 8-cell design optimised for shear, show 2.4 times higher performance when compared to hexagonal honeycombs. As demonstrated by these results, the 4-polytope-based metamaterials offer a compelling case for their adaptation in applications requiring lightweight high-performance materials.

A few mechanical metamaterial weaknesses should also be noted. The complexity involved in the fabrication of these structures usually requires highly specialised expertise, methodology and equipment. Currently, only a limited number of materials are compatible with the most commonly used manufacturing methods.
the scalability and contributing to the slow adoption of metamaterials. In addition, metamaterials are sensitive to variations in the architectured geometry. All of these mentioned weaknesses apply to the 4-polytope-based structures analysed in this work. With some of the manufacturing challenges previously discussed in Section 3.4 of Chapter 3, the fabrication of metamaterials remains one of the limiting factors for their wide-scale adoption in industrial applications. Although additive manufacturing is an enabling technology for producing complex geometries at a small scale with high precision, in general, this fabrication method does not offer an economically viable solution to upscale metamaterial production. In particular, the estimated cost of 3D printing a metamaterial array of 1 kg using the exact method proposed in this thesis, may cost between £160 and £240 depending on the production scale, while the cost of laser cutting flat sheets to be assembled into plate-lattice structures is estimated to be 20-40 times less. Although these two fabrication technologies are not directly interchangeable and offer different production rates, with 3D printing being the most suitable for low-scale prototyping and laser cutting offering the production of identical parts at much higher scales, the need for alternative manufacturing methods is evident.

Nevertheless, mechanical metamaterials have the potential to create a range of opportunities across a range of industrial applications as discussed in Section 2.4 of Chapter 2. In addition to the aforementioned sectors that were identified as the most promising sectors for the early adoption of these artificially designed structures, sports and recreation, robotics and architecture industries can also benefit from the unique properties that mechanical metamaterials can offer. Combined together with the constantly developing advanced manufacturing techniques, including but limited to additive manufacturing and fabrications using self-assembling structures, metamaterials have the potential to drive further innovation and enhance product performance. Moreover, work in this field yields lightweight, adaptive and energy-efficient structures which are required to achieve the ambitious sustainability goals of 2050. To take full advantage of the 4-polytope-based metamaterials and the unique properties these structures can offer, further work is required in this field mainly focussing on advancing the technology readiness level (TRL).

Lastly, some of the main threats associated with mechanical metamaterial development stem from the higher costs associated with the fabrication and implementation
7.4. EMERGING APPLICATION AND CHALLENGES FOR MECHANICAL METAMATERIALS

of these structures in comparison to traditional materials. This, together with com-
petition from alternative advanced material solutions is considered one of the limiting
factors for mechanical metamaterials in lower-end applications driven by cost-effective
solutions. Moreover, as the application of mechanical metamaterials is still in its early
stages, regulatory and standardization challenges are still present which may affect
the integration and acceptance of metamaterials to well-developed industries. As
previously discussed in Section 7.3, further work is required to not only adjust and
simplify the 4-polytope-based metamaterial designs but also to find substitute meth-
ods for 3D printing allowing high-precision fabrication at higher production volumes.
To summarise, mechanical metamaterials are already offering competitive solu-
tions in a range of industries regardless of the discussed weaknesses. Research in this
field has the potential to create new opportunities and tackle the identified threats
by employing unique metamaterial properties in niche applications. As shown by
this analysis, 4-polytope-based mechanical metamaterials also offer a wide range of
strengths but also have a few weaknesses that should be addressed by carrying out
future work in this field and advancing the technology readiness level.
Chapter 8

Conclusions

The work presented in this thesis explores the suitability of 4-polytope-based geometries as the basis for mechanical metamaterials and their applicability for compressive, tensile and shear loading conditions. The following sections of this chapter summarise the key findings and outputs of this work, discuss the implications and draw final remarks summarising this research work.

8.1 Validation of the thesis statement

This thesis titled “From 4-dimensional polytope projections to a new class of 3D printed mechanical metamaterials” claimed that a new class of lightweight mechanical metamaterial based on 3D projected 4-polytope geometries can be designed and manufactured to mechanically outperform conventional engineering cellular solids under static loading. This thesis statement was validated through the results presented in Chapter 4, 5 and 6 which include both simulation and experimental results benchmarked against other well-known structures.

8.2 Summary of the key findings

This work, for the first time in published literature, proposes the idea of using 3D projections of 4-polytopes as base geometries for mechanical metamaterials and throughout this thesis investigates the suitability of these structures for static compressive, tensile and shear loading applications. The results presented in Chapters 4, 5 and 6 show that the 4-polytope-based structures are highly suitable for the development of
8.3 IMPLICATIONS OF THE RESEARCH

a new class of mechanical metamaterials which perform well across a range of different loading conditions investigated in this work.

The developed methodology demonstrates that the performance of these metamaterials can not only be tailored to a specific application but also significantly enhanced in terms of specific properties related to stiffness strength by employing a GA-powered optimisation framework. In specific, the optimisation framework enhanced the specific stiffness properties by as much as 137%, 469% and 4151% for the structures developed as a part of the compression, tension and shear sets respectively.

The results presented in this thesis demonstrate that 4-polytope-based metamaterials outperform other commonly researched structures such as the gyroid and hexagonal honeycomb. To be more precise, 5, 8 and 16-cell structures surpass the gyroid structures in terms of both specific stiffness and specific yield strength in all three of the investigated loading cases. Furthermore, the respective best-performing 8-cell designs, within the compressive and tensile metamaterial sets, exceed the hexagonal honeycomb structure (in out-of-plane direction) by 17.34% and 1.05% respectively when assessed for specific yield strength. The 8-cell design optimised for shear loading demonstrates 2.4 times higher performance in specific yield strength and almost double the specific shear stiffness when compared to a hexagonal honeycomb while offering geometrical benefits due to the cubical symmetry of the unit cells. In addition to the exceptional performance of the 8-cell, the development of the shear set yielded an optimised 5-cell structure demonstrating even higher specific shear stiffness values than the 8-cell and outperforming the hexagonal honeycomb structure by 2.5 times.

Lastly, the cubically symmetrical nature of 4-polytope-based mechanical metamaterials provides significant benefits in maintaining structural stiffness and strength when subjected to multi-axial loading. The results presented in this thesis emphasise the importance of this property which is considered highly advantageous in many real-life applications and also increases the viability of 4-polytope-based metamaterial adoption within the transport and aerospace sectors.

8.3 Implications of the research

The results from this thesis provided insights into how 4-polytope-based mechanical metamaterials can be used under compressive, tensile and shear loading arrangements
and emphasised the significance of leveraging the customisable properties of mechanical metamaterials through optimisation. This work demonstrated the performance of a new class of metamaterials under standardised testing conditions and benchmarked it against other commonly researched and commercially available metamaterial structures. This is expected to elevate confidence in the use of mechanical metamaterials within the engineering industries.

During this doctoral research, nine months were spent on a research project in collaboration with a research and development company TAF composites. This added a new industrial perspective and applicability to the outcomes of this thesis. In particular, an adaptation of the models and algorithms presented in this thesis was used to develop weight-saving solutions within the wind turbine blade structures.

In addition to the direct outputs of this thesis, there were also further implications related to the peer-reviewed dissemination which will continue inspiring future work within the mechanical metamaterial research community including both, academia and industry. A complete list of papers is provided in Section 1.9 of Chapter 1. In specific, three research publications [155, 156, 157], to the best of our knowledge, are the first of their kind to demonstrate the performance of 4-polytope-based metamaterials which opens a new avenue for future research.

8.4 Final remarks

To conclude, the presented research validated the thesis statement and proved that the new class of mechanical metamaterials, analysed and discussed in this thesis, exhibits superior performance when compared to commonly researched metamaterial structures, in specific when handling compression, tension and shear loads. It introduced the concept of using 4-dimensional geometries (4-polytopes) as the basis for metamaterial unit cells by employing Schlegel diagrams to represent these shapes as wireframes in 3-dimensional space. Building on this concept, it demonstrated how these structures can be enhanced through the use of optimisation frameworks that leverage simulations, genetic algorithms and design automation. Moreover, the work demonstrated viable methods for fabrication using advanced additive manufacturing techniques and mechanical characterisation using standardised testing approaches.

This thesis showed that 4-polytope-based mechanical metamaterials can offer weight-saving benefits and an alternative to the currently used structures which is
8.4. **FINAL REMARKS**

becoming increasingly more important criteria when moving towards carbon-neutral design solutions. The main conclusions drawn from this thesis are:

- 4-polytope-based structures are highly suitable for the development of a new class of mechanical metamaterials. These structures perform well under compression, tension and shear loading, investigated in this work.

- The optimisation methodology presented in this thesis enabled the enhancement of specific stiffness properties of 4-polytope-based structures. Specifically, the specific stiffness improvements in the range of 38% - 137%, 72% - 469% and 275% - 4152% were shown for compression, tension and shear metamaterial sets respectively.

- The experimental results demonstrated that 4-polytope-based metamaterials either outperform or perform at a similar level to the gyroid and the hexagonal honeycomb structures in terms of specific stiffness and strength in all investigated loading conditions.

- All 4-polytope-based mechanical metamaterials were shown to have cubically symmetrical geometrical arrangements. This was found beneficial for the structural stiffness and strength of these structures and for enhancing metamaterial performance in multi-axial loading scenarios.

- The 8-cell structures were found to perform best within the metamaterial sets developed for compression and tension in terms of specific stiffness and strength.

- Within the 4-polytope-based metamaterials developed for shear loading, the 5-cell has the highest specific shear stiffness while the structure with the highest specific shear strength is the 8-cell.

- To summarise, the 8-cell was identified as the top-performing structure under the investigated static loading modes, specifically tension, compression and shear.
Appendix A

Parametric design variables
Table A.1: Compression set. Parametric design variable table summarising the specified range used in design space exploration and optimum parameter values (100% of total optimisation - case (iv)) obtained using the optimisation algorithm. The full set of raw optimisation data is also made available on the Edinburgh Data Share website [20].

<table>
<thead>
<tr>
<th>5-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>1.00 - 2.70</td>
<td>1.85</td>
<td>1.78</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.05 - 0.20</td>
<td>0.13</td>
<td>0.10</td>
</tr>
<tr>
<td>C Corner distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
<td>1.12</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
<td>0.13</td>
</tr>
<tr>
<td>E Corner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
<td>0.21</td>
</tr>
<tr>
<td>F Outer corner round</td>
<td>0.20 - 0.50</td>
<td>0.35</td>
<td>0.27</td>
</tr>
<tr>
<td>G Inner triangle size</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
<td>0.29</td>
</tr>
<tr>
<td>H Outer shell thickness</td>
<td>0.10 - 0.60</td>
<td>0.35</td>
<td>0.54</td>
</tr>
<tr>
<td>I Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>1.38</td>
</tr>
<tr>
<td>J Outer shell round</td>
<td>0.10 - 2.00</td>
<td>1.05</td>
<td>0.22</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole round radius</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
<td>1.40</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>2.00 - 3.80</td>
<td>2.90</td>
<td>2.07</td>
</tr>
<tr>
<td>C Inner edge round radius</td>
<td>0.05 - 0.50</td>
<td>0.28</td>
<td>0.24</td>
</tr>
<tr>
<td>D Inner cube size</td>
<td>2.00 - 4.20</td>
<td>3.10</td>
<td>3.48</td>
</tr>
<tr>
<td>E Outer wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
<td>0.16</td>
</tr>
<tr>
<td>F Inner cube wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
<td>0.17</td>
</tr>
<tr>
<td>G Outer edge round radius</td>
<td>0.10 - 1.20</td>
<td>0.65</td>
<td>0.45</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
<td>2.91</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.05 - 0.45</td>
<td>0.25</td>
<td>0.38</td>
</tr>
<tr>
<td>C Inner triangle size</td>
<td>2.50 - 4.00</td>
<td>3.25</td>
<td>2.50</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>0.10 - 0.25</td>
<td>0.18</td>
<td>0.10</td>
</tr>
<tr>
<td>E Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>0.91</td>
</tr>
<tr>
<td>F Outer shell round</td>
<td>0.30 - 0.60</td>
<td>0.45</td>
<td>0.31</td>
</tr>
<tr>
<td>G Outer shell thickness</td>
<td>0.10 - 0.80</td>
<td>0.45</td>
<td>0.75</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>24-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>4.35 - 5.50</td>
<td>4.93</td>
<td>4.49</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>0.96</td>
</tr>
<tr>
<td>C Inner triangle size</td>
<td>1.00 - 4.00</td>
<td>2.50</td>
<td>1.76</td>
</tr>
<tr>
<td>D Inner triangle round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
<td>0.54</td>
</tr>
<tr>
<td>E Projection angle</td>
<td>0.10° - 10.00°</td>
<td>5.05°</td>
<td>8.97°</td>
</tr>
<tr>
<td>F Outer shell round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
<td>0.67</td>
</tr>
<tr>
<td>G Inner wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.35</td>
</tr>
<tr>
<td>H Middle wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.25</td>
</tr>
<tr>
<td>I Outer wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.20</td>
</tr>
</tbody>
</table>
Table A.2: Tension set. Parametric design variable table detailing the specified parameter range, starting value and the optimum value obtained using the optimization method (100% of total optimization - case (iv)). The full raw optimization dataset is available on the Edinburgh Data Share website [21].

<table>
<thead>
<tr>
<th>5-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Drain hole distance</td>
<td>1.00 - 2.70</td>
<td>1.85</td>
</tr>
<tr>
<td>B</td>
<td>Drain hole radius</td>
<td>0.05 - 0.20</td>
<td>0.13</td>
</tr>
<tr>
<td>C</td>
<td>Corner distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
</tr>
<tr>
<td>D</td>
<td>Inner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
</tr>
<tr>
<td>E</td>
<td>Corner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
</tr>
<tr>
<td>F</td>
<td>Outer corner round</td>
<td>0.20 - 0.50</td>
<td>0.35</td>
</tr>
<tr>
<td>G</td>
<td>Inner triangle size</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
</tr>
<tr>
<td>H</td>
<td>Outer shell thickness</td>
<td>0.10 - 0.60</td>
<td>0.35</td>
</tr>
<tr>
<td>I</td>
<td>Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
</tr>
<tr>
<td>J</td>
<td>Outer shell round</td>
<td>0.10 - 2.00</td>
<td>1.05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Drain hole round radius</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
</tr>
<tr>
<td>B</td>
<td>Drain hole radius</td>
<td>2.00 - 3.80</td>
<td>2.90</td>
</tr>
<tr>
<td>C</td>
<td>Inner edge round radius</td>
<td>0.05 - 0.50</td>
<td>0.28</td>
</tr>
<tr>
<td>D</td>
<td>Inner cube size</td>
<td>2.00 - 4.20</td>
<td>3.10</td>
</tr>
<tr>
<td>E</td>
<td>Outer wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
</tr>
<tr>
<td>F</td>
<td>Inner cube wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
</tr>
<tr>
<td>G</td>
<td>Outer edge round radius</td>
<td>0.10 - 1.20</td>
<td>0.65</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Drain hole distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
</tr>
<tr>
<td>B</td>
<td>Drain hole radius</td>
<td>0.05 - 0.45</td>
<td>0.25</td>
</tr>
<tr>
<td>C</td>
<td>Inner triangle size</td>
<td>2.50 - 4.00</td>
<td>3.25</td>
</tr>
<tr>
<td>D</td>
<td>Inner wall thickness</td>
<td>0.10 - 0.25</td>
<td>0.18</td>
</tr>
<tr>
<td>E</td>
<td>Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
</tr>
<tr>
<td>F</td>
<td>Outer shell round</td>
<td>0.10 - 2.00</td>
<td>1.05</td>
</tr>
<tr>
<td>G</td>
<td>Outer shell thickness</td>
<td>0.10 - 0.80</td>
<td>0.45</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>24-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Drain hole distance</td>
<td>4.35 - 5.50</td>
<td>4.93</td>
</tr>
<tr>
<td>B</td>
<td>Drain hole radius</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
</tr>
<tr>
<td>C</td>
<td>Inner triangle size</td>
<td>1.00 - 4.00</td>
<td>2.50</td>
</tr>
<tr>
<td>D</td>
<td>Inner triangle round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
</tr>
<tr>
<td>E</td>
<td>Projection angle</td>
<td>0.10° - 10.00°</td>
<td>5.05°</td>
</tr>
<tr>
<td>F</td>
<td>Outer shell round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
</tr>
<tr>
<td>G</td>
<td>Inner wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
</tr>
<tr>
<td>H</td>
<td>Middle wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
</tr>
<tr>
<td>I</td>
<td>Outer wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
</tr>
</tbody>
</table>
Table A.3: Shear set. A list of parametric design variables for each 4-polytope metamaterial including specified parameter range, starting value and the optimum value (100% of total optimization - case (iv)) found using the optimisation algorithm. The full raw optimization dataset is available on the Edinburgh Data Share website [22].

<table>
<thead>
<tr>
<th>5-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>1.00 - 2.70</td>
<td>1.85</td>
<td>1.81</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.05 - 0.20</td>
<td>0.13</td>
<td>0.15</td>
</tr>
<tr>
<td>C Corner distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
<td>1.21</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
<td>0.05</td>
</tr>
<tr>
<td>E Corner wall thickness</td>
<td>0.05 - 0.30</td>
<td>0.18</td>
<td>0.09</td>
</tr>
<tr>
<td>F Outer corner round</td>
<td>0.20 - 0.50</td>
<td>0.35</td>
<td>0.21</td>
</tr>
<tr>
<td>G Inner triangle size</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
<td>0.16</td>
</tr>
<tr>
<td>H Outer shell thickness</td>
<td>0.10 - 0.60</td>
<td>0.35</td>
<td>0.16</td>
</tr>
<tr>
<td>I Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>0.94</td>
</tr>
<tr>
<td>J Outer shell round</td>
<td>0.10 - 2.00</td>
<td>1.05</td>
<td>1.78</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole round radius</td>
<td>0.10 - 1.50</td>
<td>0.80</td>
<td>0.66</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>2.00 - 3.80</td>
<td>2.90</td>
<td>2.80</td>
</tr>
<tr>
<td>C Inner edge round radius</td>
<td>0.05 - 0.50</td>
<td>0.28</td>
<td>0.14</td>
</tr>
<tr>
<td>D Inner cube size</td>
<td>2.00 - 4.20</td>
<td>3.10</td>
<td>2.50</td>
</tr>
<tr>
<td>E Outer wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
<td>0.11</td>
</tr>
<tr>
<td>F Inner cube wall thickness</td>
<td>0.10 - 0.20</td>
<td>0.15</td>
<td>0.10</td>
</tr>
<tr>
<td>G Outer edge round radius</td>
<td>0.10 - 1.20</td>
<td>0.65</td>
<td>0.16</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>1.00 - 5.00</td>
<td>3.00</td>
<td>1.43</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.05 - 0.45</td>
<td>0.25</td>
<td>0.42</td>
</tr>
<tr>
<td>C Inner triangle size</td>
<td>2.50 - 4.00</td>
<td>3.25</td>
<td>2.63</td>
</tr>
<tr>
<td>D Inner wall thickness</td>
<td>0.10 - 0.25</td>
<td>0.18</td>
<td>0.15</td>
</tr>
<tr>
<td>E Outer shell width</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>0.82</td>
</tr>
<tr>
<td>F Outer shell round</td>
<td>0.10 - 2.00</td>
<td>1.05</td>
<td>1.11</td>
</tr>
<tr>
<td>G Outer shell thickness</td>
<td>0.10 - 0.80</td>
<td>0.45</td>
<td>0.14</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>24-cell</th>
<th>Specified range</th>
<th>Starting value</th>
<th>Optimum value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A Drain hole distance</td>
<td>4.35 - 5.50</td>
<td>4.93</td>
<td>4.69</td>
</tr>
<tr>
<td>B Drain hole radius</td>
<td>0.50 - 2.00</td>
<td>1.25</td>
<td>0.68</td>
</tr>
<tr>
<td>C Inner triangle size</td>
<td>1.00 - 4.00</td>
<td>2.50</td>
<td>2.67</td>
</tr>
<tr>
<td>D Inner triangle round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
<td>0.55</td>
</tr>
<tr>
<td>E Projection angle</td>
<td>0.10° - 10.00°</td>
<td>5.05°</td>
<td>2.47°</td>
</tr>
<tr>
<td>F Outer shell round</td>
<td>0.20 - 0.80</td>
<td>0.50</td>
<td>0.33</td>
</tr>
<tr>
<td>G Inner wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.39</td>
</tr>
<tr>
<td>H Middle wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.26</td>
</tr>
<tr>
<td>I Outer wall thickness</td>
<td>0.20 - 0.40</td>
<td>0.30</td>
<td>0.26</td>
</tr>
</tbody>
</table>
Appendix B

Progressive optimisation outputs
Figure B.1: Progressive optimisation of the compressive metamaterial set with each column showing the geometrical arrangement at a different stage. The full dataset is made available on the Edinburgh Data Share website [20].
Figure B.2: Progressive optimisation of the tensile metamaterial set with each column showing the geometrical arrangement at a different stage. The full dataset is made available on the Edinburgh Data Share website [21].
Figure B.3: Progressive optimisation of the shear metamaterial set with each column showing the geometrical arrangement at a different stage. The full dataset is made available on the Edinburgh Data Share website [22].
Appendix C

Inside Front Cover: Advanced Engineering Materials
Figure C.1: Inside Front Cover: *Advanced Engineering Materials*. 
References


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES


REFERENCES

manufacturing (3D printing): A review of materials, methods, applications and 


[98] Y. H. Zhang, X. M. Qiu, and D. N. Fang, “Mechanical Properties of two 
novel planar lattice structures,” International Journal of Solids and Structures, 

[99] F. Cote, V. S. Deshpande, N. A. Fleck Volume, and N. A. Fleck, “The shear 
response of metallic square honeycombs,” Journal of Mechanics of Materials 

[100] F. Côté, V. S. Deshpande, N. A. Fleck, and A. G. Evans, “The compressive and 
shear responses of corrugated and diamond lattice materials,” International 

[101] CEL COMPONENTS S.R.L., “Polypropylene honeycomb core PP8-120T30 
poliprop_P880_Rev1_uk.pdf.

Surfaces and Related Geometry: From Biological Structures to Self-Assembled 

two-dimensional bending can extraordinarily stiffen thin sheets,” Scientific Re-
ports, vol. 6, no. 1, pp. 1–6, 7 2016.


[105] D. W. Abueidda, M. Bakir, R. K. Abu Al-Rub, J. S. Bergström, N. A. Sobh, 
and I. Jasiuk, “Mechanical properties of 3D printed polymeric cellular materials 
with triply periodic minimal surface architectures,” Materials and Design, vol. 

154
REFERENCES


REFERENCES


[125] C. Morris and C. Seepersad, “Efficient identification of promising regions in high-dimensional design spaces with multilevel materials design applications,”
REFERENCES


REFERENCES


REFERENCES


REFERENCES


161
REFERENCES


